



A coupled Volume-of-Fluid and Lagrangian Point-Particle approach for investigating the plain liquid jet in crossflow atomization

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ABSTRACT

The atomization of a liquid jet in crossflow is revisited for the density ratio corresponding to conventional Jet A-1 aviation fuel by numerical simulations. To correctly capture the large range of spatial scales involved, the coupled methods of momentum conserving Volume-of-Fluid and Lagrangian Particle Tracking methods are used. Both solvers are combined via momentum coupling and two-way droplet conversion. Additionally, we take advantage of Adaptive Mesh Refinement to save computation time. The Lagrangian method is free from coalescence and breakup models, therefore a global criterion is applied to avoid droplet transfer from the VOF solver to the Lagrangian solver in the region with a high number of coalescence events. To achieve this, a new post-processing method for identifying coalescence and disintegration of droplets is described. The Lagrangian method is validated regarding single droplet trajectories, and a qualitative validation of the Euler–Lagrange conversion is presented. Two different sets of inflow velocities for the gaseous and liquid phases are investigated. The results obtained with the coupled Euler–Lagrange method show a good agreement with those from pure Eulerian VOF simulations, regarding droplet size and velocity distributions and column breakup point. Jet penetration is validated, and the Sauter Mean Diameter is close to experimental correlations. A significant reduction of computational cost is achieved by the coupling to the Lagrangian method.

1. Introduction

Drop dispersion in form of sprays is present in many natural phenomena and industrial applications. In aero-engines, the atomization of the liquid fuel is key to an efficient combustion and to low emissions. Increased fuel area-to-volume ratio achieved with small droplets is desired to enhance vaporization and therefore rapid mixing of fuel and oxidizer in the gas phase. Further, homogeneous mixing avoids temperature peaks, which augment emissions. Airblast nozzles are ideally suited for atomizing liquid fuels in continuous-flow combustion systems, such as gas turbines in the energy and aviation sector. Certain nozzles in that category rely on the atomization of a plain jet in a crossflow to generate micron-size droplets. They find widespread application in modern aero-engine combustion systems, as for example the twin annular premixing swirler (TAPS) of General Electric GENx turbofan engine. More generally, Lean Premixed Prevaporized combustors with a staged lean combustion technology are able to reduce NO_x emissions very effectively. Fuel is injected into the primary stage at multipoint ports and is rapidly atomized by the crossflow air provided by the primary axial swirler [1,2].

Atomization of a liquid jet in crossflow (JICF) involves several breakup mechanisms. The primary breakup of the liquid column as a whole results from the growth of axial instability waves on the jet surface. Simultaneously, ligament shedding is observed on the lateral surface and can be described by two different models. The boundary layer stripping model [3] assumes that the liquid mass is removed from the viscous boundary layer inside the jet. In the Kelvin–Helmholtz model [4,5], the ligament pinch-off results from lateral instability waves. All the liquid fragments formed undergo additional secondary breakup processes. A detailed description of droplet features and formation mechanisms can be found in the comprehensive literature review by Broumand and Birouk [6], together with regime maps and numerous correlations that describe the trajectory, penetration and column breakup position of a plain liquid jet. The authors give a list of unresolved questions concerning turbulence and cavitation, operating conditions at high pressure and temperature, or internal injector geometry and injection angle.

High-fidelity simulations can provide insight into the complex disintegration phenomena that are difficult to observe experimentally. Detailed Numerical Simulations (DNS) with interface capturing methods such as Volume-of-Fluid (VOF), Level-Set or coupled Level-Set and

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VOF (CLSVOF) are optimal tools to simulate the liquid disintegration process in fine detail in a limited domain. We note that the CLSVOF method combines the benefits from the level set and VOF methods, offering both the geometrical accuracy and mass conservation. Recent investigations investigate the physics of the liquid jet in crossflow atomization for different parameter regimes [7–9]. However, they often reach the limits of computing capacity due to the large range of length and time scales involved. An alternative approach is to complement these methods with subgrid-scale models (SGS) to address the multi-scale challenge and enable simulations of larger domains. These models include Lagrangian Particle Tracking (LPT) and Large Eddy Simulations (LES). The Lagrangian method consists in modeling the trajectories of the small droplets in the gas flow using the point-droplet approximation. It offers the double advantage of saving computation time and enabling model-based trajectory prediction when Euler resolution is insufficient. In the Large Eddy Simulations, the unresolved and filtered subgrid-scale terms are modeled. Recently, Sun et al. [10] extended the VOF method by incorporating the SGS term into the VOF transport equation, creating a coupled LES-VOF framework to capture the interaction between turbulence and interfaces. Applying this framework to simulate the atomization of a liquid jet in crossflow, they observed an elongated liquid core, prolonged ligament breakup and therefore delayed column breakup. Furthermore, the use of LPT and Adaptive Mesh Refinement (AMR) in conjunction with their approach led to significant reduction in computational costs. However, this method is only able to increase the accuracy for surface topology changes larger than the LES cutoff, whereas smaller structures still remain unresolved.

A brief overview of the publications on coupled Eulerian–Lagrangian methods is given in the following. Herrmann uses the refined level set grid method in a block-structured Adaptive Mesh Refinement (AMR) environment to investigate the atomization of a turbulent liquid jet in the crossflow configuration [11] injected into still compressed air under diesel engine conditions [12]. Small and nearly spherical drops are identified and transferred, after testing droplet volume and the aspect ratio. Moreover, as small droplets are more stable regarding breakup due to the higher surface tension force compared to the aerodynamic force, they note that, the Weber number, Capillary number, or drop internal fluctuation kinetic energy can also be used to indicate further breakup of the droplet. In subsequent work, the same methods are used to investigate the primary atomization of a turbulent liquid jet in the crossflow [13]. The impact of density ratio is addressed in two following publications [14,15]. Turbulence in the single phase regions of the flow is modeled using a dynamic Smagorinsky large eddy simulation model, and inflow boundary conditions are taken from a precomputed LES pipe flow simulation. The grid dependency of resulting jet penetration and droplet size distribution is discussed. The nature of the windward instability waves is also discussed with the help of proper orthogonal decomposition.

Li et al. [16] introduce the additional criterion of local concentration in their Coupled Level Set and Volume-of-Fluid method (CLSVOF) algorithm to quantify the amount of liquid phase in the region around the droplet to be transferred. Below a critical value of this parameter, a dilute spray region can be assumed where collisions can be neglected. They consider only quasi-steady forces, and use the drag coefficient for a rigid sphere. The point-droplets are only one-way coupled to the flow through their relative velocity with respect to the gas phase. Their results of the atomization of a liquid jet in crossflow did not converge, whereas the droplet size distributions for two impinging jet showed good agreement with experiments. Tomar et al. [17] studied primary atomization with a VOF algorithm implemented in Gerris coupled with a two-way coupling Lagrangian particle-tracking model. The momentum source term in the Navier–Stokes equations is smoothed using a Gaussian distribution function. Point-droplets can be converted back into VOF based on their proximity to the VOF interface. They give the extensive list of the forces acting on point-droplets: the inertial, added-mass and lift force. To account for droplet-droplet interactions,

a hard-sphere collision model is applied. After the successful validation with a set of test cases, the algorithm was applied to the atomization of a liquid jet by a high-speed coaxial gas flow. Ling et al. [18] investigated the primary atomization of a pulsed liquid jet with a VOF method as implemented in the code ParisSimulator, as well as gas-assisted atomization. In the later case, fast air is injected on top of a slower liquid jet, with both inflow velocities applied in the same direction. They retain unsteady forces, pressure-gradient and added-mass force, although they are negligible for high density ratios and employ the standard drag correlation for solid particle. The two-way coupling force exerted by the Lagrangian droplets to the resolved flow is also distributed with a Gaussian function. Resolved droplets are qualified for a conversion to Lagrangian Point-Particle (LPP) representation, if their size is smaller than 4–6 cell sizes, for aspect ratio near one, and far away from the resolved interface. The undisturbed flow-field has to be restored after droplet removal. This means that during the inverse conversion back to resolved droplets, the momentum of both the drop and the virtual fluid accompanying the droplet must be added back. A good agreement with experiments was observed. Zuzio et al. [19] investigated a planar liquid sheet atomization combining interface-capturing scheme based on coupled level-Set/Volume-of-fluid method (CLSVOF) with adaptive mesh refinement and LPP models. They propose a smooth transition between the Eulerian and the Lagrangian droplet modeling. They distinguish between small and medium Lagrangian droplets for droplets sizes smaller and greater than the local mesh size, respectively. They indicate that medium droplets arising immediately after conversion need an intermediate treatment between pure Eulerian and Lagrangian drag force model. The flow still sees a liquid inclusion of the size of the medium droplet. Later in time, when the grid is coarser, the point-droplet assumption and drag-force model is valid. The validation case of a droplet splashing on a liquid free surface is presented [19]. Chéron et al. [20] achieve more accurate results for poorly resolved droplets by two-way coupling a Lagrangian method with the CLSVOF method. They take into account the local flow disturbance induced by the Lagrangian droplets to obtain the flow velocity around them [21], and validated the self-disturbance correction technique with the final velocity of a sedimented free-falling droplet. They solved the mass inconsistency shown in the Lagrangian to Eulerian transformation searching for the radius of reconstruction that minimizes the difference between the reconstructed Eulerian and the Lagrangian droplet. Their criterion for transferring droplets are the numerical resolution, the distance to other droplets and the morphology i.e. the aspect ratio and irregularity. However, the simulation with the two way Lagrangian coupling is computationally expensive, so that the computational cost for the liquid jet in crossflow simulations is only slightly reduced when applying the one-way coupling.

In the present work, the atomization of conventional fuel Jet A-1 in the jet in crossflow configuration is investigated. The large-scale interface is tracked with the Basilisk momentum conserving Volume-of-Fluid method (basilisk.fr [22–24]). The small liquid structures, which are not so small as to be meaningless in the Eulerian framework, are transferred to the Lagrangian method, leading to a more accurate prediction of their trajectory. The Lagrangian method is inspired from previous state-of-the-art implementations, consistent with Basilisk language and AMR, and parallelized in order to allow computation in a domain large enough to cover the complete spray evolution, including primary and secondary breakup processes. The first goal of the present work is to achieve a good agreement with results from pure VOF simulations regarding droplet distributions. A special care is dedicated to the identification of coalescence and breakup events in DNS simulations, and to the definition of a global droplet conversion criteria. The coupled Lagrangian and VOF method is validated, by comparing droplet distributions, jet penetration, and breakup points against pure VOF simulations and against experimental results. While the accuracy of the Lagrangian tracking method is guaranteed by the choice of

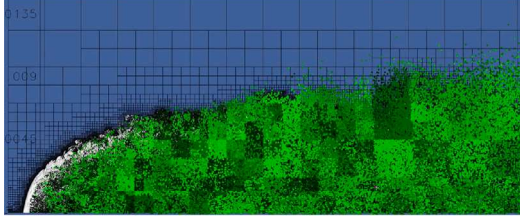


Fig. 1. Atomization of a kerosene (Jet A-1) jet in crossflow and AMR up to a maximum level of refinement of value 12 (defined in Section 2.1). The snapshot is captured at $t = 0.495$ ms. The VOF interface (white), and the Lagrangian droplets (green) are shown. The square domains are computed by different processors using different shades of green when displaying the Lagrangian droplets. A slice of the adapted mesh is also represented. The Lagrangian method is performed without the criteria concerning the coalescence events explained in Section 2.3.2.

droplet conversion criteria, the second aim was to track a large part of the droplets in a Lagrangian way to reduce the computation effort.

This manuscript is organized as follows. It first details the methods used and further implemented in the flow solver Basilisk. After a brief overview of the Volume-of-Fluid method, a detailed description of the Lagrangian method implemented in the Basilisk environment is presented thereafter. In the second part, we present the parameters of the two jet-in-crossflow cases investigated in this study, considering only pure VOF simulations. The degree of convergence of pure VOF simulations conducted until the quasi stationary state is discussed. A quantitative validation using experimental results is performed and convergence regarding droplet distributions is evaluated. In the third part, we discuss the results obtained from coupling VOF with the Lagrangian method. A qualitative validation is performed through the visualization of droplet trajectories shortly after Euler–Lagrange conversion. For quantitative validation, single droplets of varying resolution are analyzed. Subsequently, the location of coalescence events is given in order to define the minimal distance from the coherent jet for which the Euler to Lagrange conversion is applied. Differences in droplets size and velocity distributions between pure VOF and coupled simulations are analyzed, highlighting improvements from the coalescence criterion. Jet penetration is validated, and the location of the breakup point is discussed. Finally, we specify how much computation time is saved by coupling to the Lagrangian method and the coarser resolution of the velocity field in the bulk phases.

2. Governing equations and numerical implementation

The simulations are mainly conducted with the open source software Basilisk for two-phase flow simulations based on the Volume-of-Fluid method. The fully resolved droplets, which do not undergo any further breakup are transferred to the LPP solver. The quasi-steady force exerted on the Lagrangian droplets by the undisturbed gas-field is modeled. Moreover, we compute the additional source term in the Navier–Stokes equations which is due to the spray. It is derived from the change in momentum of the point-droplets in the Lagrangian framework and completes the two-way-coupling between both solvers. The point-droplets located close to the dispersed phase in the DNS are allowed to return back to resolved droplets in DNS. Droplet collisions, merging and disintegration are not accounted for in the Lagrangian framework. We use the AMR technique offered by Basilisk in order to save computational time. A snapshot of the simulation combining all these methods is shown in Fig. 1. The resolved interface and the point-droplets are both shown.

2.1. Overview of the volume-of-fluid method

For the resolved flow, the Navier–Stokes equations for incompressible two-phase interfacial flows at isothermal conditions are solved:

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot [(\rho \mathbf{u}) \otimes \mathbf{u}] = -\nabla p + \nabla \cdot (2\mu \mathbf{D}) + \mathbf{f}_\sigma + \rho \mathbf{g} + \Phi^p(\mathbf{x}) \quad (1)$$

with $\mathbf{D} = [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]/2$ the deformation tensor, $\mathbf{f}_\sigma$ the volumetric surface tension, $\rho \mathbf{g}$ the gravity force [23,25], and ρ , $\mathbf{u}$, p , μ being respectively the density, the velocity, the pressure, and the dynamic viscosity. In the case of coupled Euler–Lagrange simulations, a source term $\Phi^p(\mathbf{x})$ generated by the dispersed phase simulated using the Lagrangian approach is included (see Section 2.3.4).

A finite volume formulation is adopted, with the fields representing cell averages. The timestep is controlled by the Courant–Friedrichs–Lewy (CFL) stability condition. Time discretization follows a classical fractional-step projection method, where densities are lagging velocities by half a timestep. The curvature κ needed for the surface tension $\mathbf{f}_\sigma = \sigma \kappa \delta_s \mathbf{n}$ is calculated with the Height Function method [23]. A Poisson equation for the pressure is solved by a multigrid method.

The interface is tracked with the VOF method. Mass conservation together with incompressibility lead to the following transport equation for the volume fraction of fluid f :

$$\partial_t f + \nabla \cdot (f \mathbf{u}) = 0 \quad (2)$$

The volume fraction varies between the values 0 and 1 for cells completely encased in the gas phase and in the liquid phase respectively. To avoid numerical diffusion, the interface is reconstructed with the piecewise linear interface calculation (PLIC) method [26]. A split advection method according to Weymouth and Yue [27] based on the geometrical fluxes cut by the plane interface is conducted. The computed fluxes for advection are also used for momentum convection to achieve momentum conservation. This momentum-conserving Volume-of-Fluid (MCVOF) method was introduced by Fuster and Popinet [28].

In this work, we use Basilisk adaptive octree grids introduced and explained in detail in [24,29]. The cartesian grid structure is tree-based and can vary over the course of the simulation based on the evolution of the volume fraction of liquid and velocity fields. There is a hierarchy of cells at different levels of refinement, and the level of refinement l is related to the cell size by $\Delta(l) = D_0/2^l$. The procedure to determine which cells require refinement or coarsening is based on the estimation of an absolute error in the field values, called error tolerance in the following. For sake of comprehension of the technical details of the present work, we mention that leaf cells are the finest cells in the octree grid formalism.

For pure VOF simulations, the maximum level of refinement for adaption to the velocity fluctuations and those of the liquid volume fraction is the same. The reason is, that these simulations serve as a reference for comparison with results from coupling with the Lagrangian method. We have carried them out as accurately as possible.

2.2. Lagrangian particle tracking

The differential equations for droplet position $\mathbf{x}_p$ and velocity $\mathbf{u}_p$ solved along point-droplet trajectories read:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p \quad (3)$$

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{a}_d + \left(1 - \frac{\rho_g}{\rho_l}\right) \mathbf{g} \quad (4)$$

The acceleration is due to the drag and gravity forces.

We model the quasi-steady force with the drag:

$$\mathbf{a}_d = \frac{3}{4} \frac{c_d}{d_p} \frac{\rho_g}{\rho_l} |\mathbf{u}_{rel}| \mathbf{u}_{rel} \quad (5)$$

$\mathbf{u}_{rel} = \mathbf{u}_f - \mathbf{u}_p$ being the undisturbed velocity of the gas flow $\mathbf{u}_f$ relative to the droplet velocity. $\mathbf{u}_f$ is evaluated at droplet position $\mathbf{x}_p$ with

trilinear interpolation from the velocity field $\mathbf{u}$ solved within the VOF method. We neglect the effect of the internal flow on the drag, and use the drag coefficient c_d for solid spheres given as a function of droplet Reynolds number $Re_p = \frac{d_p \rho_g |\mathbf{u}_{rel}|}{\mu_g}$ in different regimes (see the expressions for it in the book of Acrivos [30] p.112). For the first approximation, considering the drag coefficient of a solid sphere is justified for $\mu_l \gg \mu_g$.

The unsteady contributions from the inertial force, the added-mass force, the lift force, and the Basset-history force are not considered. According to Bagchi and Balachandar [31] and regarding the particle acceleration, the ratio of added mass force to the quasi-steady force is of the order of $1/(\rho_l/\rho_g + C_M) \approx 0.01$ for our case. C_M is the added mass term, which is equal to $1/2$ for a sphere and is of the order of 1 in general. The ratio of Basset-history force to the quasi-steady force is then of the order of $1/\sqrt{\rho_l/\rho_g + C_M} \approx 0.1$, which is non-negligible but not accounted for simplicity. For large density ratios $\frac{\rho_l}{\rho_g}$, Ling et al. [32] used a more rigorous evaluation of the particle response to a range of turbulent scales to show that the added-mass and history force become relevant when the droplet size is in the range of the Kolmogorov scale [32].

For the time discretization, a fixed Lagrangian time step $dt_{Lag} = 5 \times 10^{-6}$ s is used, which is about 200 times larger than the DNS time step. The choice is justified in Section 3.2. We note that Sun et al. [10] also use a fixed timestep, they check the conversion criteria every 40 timesteps in the Euler framework. Hence, the coupling with the staggered in time discretization of the Basilisk solver is simplified, as we can assume that the volume fractions and velocities are calculated at the same time.

The droplet velocity is obtained from the analytical solution of Eq. (4), where the relaxation time $\tilde{\tau}_p$ is calculated at the mean droplet velocity $\bar{\mathbf{u}}_p$ during the Lagrangian time step.

$$\tilde{\tau}_p = \frac{4d_p \rho_l}{3c_d \left(|\mathbf{u}_f - \bar{\mathbf{u}}_p| \right) \rho_g |\mathbf{u}_f - \bar{\mathbf{u}}_p|} \quad (6)$$

The differential solution for droplet velocity and its solution read:

$$\begin{aligned} \frac{d\mathbf{u}_p}{dt} &= \frac{\mathbf{u}_{rel}}{\tilde{\tau}_p} + \left(1 - \frac{\rho_g}{\rho_l} \right) \mathbf{g} \\ \mathbf{u}_p(t + dt_{Lag}) &= \mathbf{u}_p(t) + [1 - \exp(-dt_{Lag}/\tilde{\tau}_p)] \\ &\quad \cdot [\mathbf{u}_f - \mathbf{u}_p(t) + \tilde{\tau}_p(1 - \rho_g/\rho_l)\mathbf{g}] \end{aligned}$$

The mean droplet velocity in the interval $[t, t + dt_{Lag}]$ is calculated from this solution and following expression is obtained:

$$\mathbf{u}_f - \bar{\mathbf{u}}_p = (\mathbf{u}_f - \mathbf{u}_p(t)) \left(\frac{1 - \exp(-dt_{Lag}/\tilde{\tau}_p)}{dt_{Lag}/\tilde{\tau}_p} \right)$$

An iterative procedure is applied to determine $\bar{\mathbf{u}}_p$ from the latter expression and Eq. (6).

In the VOF method, no-slip boundary conditions prevail at the bottom wall, and the VOF variable is set to zero at the wall, corresponding to a perfect hydrophobic surface boundary condition. These boundary conditions are consistent with the elastic droplet-wall collision assumed for the Lagrangian droplets, and allow a better comparison between pure VOF simulations and those coupled with the Lagrangian method.

2.3. Eulerian-Lagrangian coupling

2.3.1. Identification of the droplets and their parameters

The coherent isolated liquid structures are identified with the Basilisk tag function, which tags connected regions. A unique index is associated to all the cells which belong to the same structure. We note that only cells with liquid volume fractions greater than a given threshold value, set to 10^{-4} , are used for identification. Therefore, droplet parameters are deduced easily: i.e. droplet centroid $\mathbf{x}_p$, volume

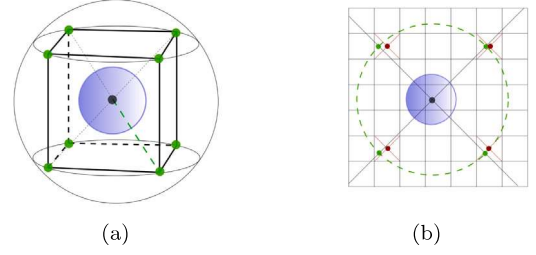


Fig. 2. Interpolation of the undisturbed flow velocity. First, 8 points (marked with green dots) at a distance $1.5 d_p$ from the droplet centroid are determined (a). Then, the center of the cells (marked with red dots) containing these points are determined ((b) shows the 2D visualization). The velocity values at these cell centers are used for interpolation.

V_p and velocity $\mathbf{u}_p$. Droplet diameter $d_p = (6V_p/\pi)^{1/3}$ is calculated assuming a spherical droplet. All these parameters are then assigned to the Lagrangian droplets. We note that $\mathbf{u}_p$ is the mean velocity over the cells filled with liquid, which means that inner circulations are neglected. Moreover, the aspect ratio $\epsilon = r_{max}/r_{min}$ is estimated. We determine r_{max} and r_{min} as the maximum and minimum distance of droplet centroid $\mathbf{x}_p$ to the barycenter of the interface among all mixed cells, respectively.

In order to calculate the Weber number criterion, the undisturbed flow velocity in the vicinity of the droplet, denoted as $\mathbf{u}_f$, has to be determined (see Eq. (7)). The latter is required to estimate droplet velocity relative to the gas phase velocity $\mathbf{u}_{rel}$. In practice, the approximate undisturbed flow velocity $\mathbf{u}_f$ is evaluated at droplet centroid location, from interpolating 8 velocity values at as many cell centers containing points located at a distance $1.5 d_p$ from the droplet centroid. These points are the corners of a cube with edges oriented along the coordinate axis (see Fig. 2). We require that the cells containing the points are first or second neighbors of the leaf cell where droplet centroid is located, or of a parent cell of this leaf cell. All of the 8 cells are at the same level of refinement, and we take the highest matching level. Doing so, we avoid any costly communication of the droplet location in parallel runs as field values are available in Basilisk up to second neighbors of each cell at any level located in the domain of a given processor. According to Ling et al. [18], the Lagrangian droplet represents not only the momentum of the droplet, but also the momentum of the unresolved perturbed flow around the droplet, so that the momentum of the overall system is conserved.

2.3.2. From resolved droplets in DNS to point-droplets in Lagrange formalism

The first criterion for transferring droplets is their degree of resolution. Only droplets with a diameter exceeding twice the smallest cell size are transferred. The reason for this is that the DNS droplets with a diameter below this cutoff are under-resolved (see Section 3.2.1). Secondly, we consider only slightly distorted droplets with aspect ratio $r_{max}/r_{min} < 2.5$. Consequently, ligaments and strongly distorted fragments are excluded, as they might experience secondary breakup. This cutoff value of 2.5 is not very restrictive compared with other values related to deformation criteria found in the literature [16,19,33], but droplet stability regarding breakup is also assessed with the Weber number and the coalescence criterion introduced below. The aspect ratio is easy to compute and utilized for preselecting the droplets. Actually, the criterion for assessing the absence of drop secondary breakup is to examine whether the droplet's Weber number satisfies the required condition:

$$We = \frac{\rho_g d_p |\mathbf{u}_{rel}|^2}{\sigma} < 12 \quad (7)$$

This value is recommended by Pilch and Erdman [34] and Hwang et al. [35] for low viscosity liquids with the Ohnesorge number $Oh < 0.1$

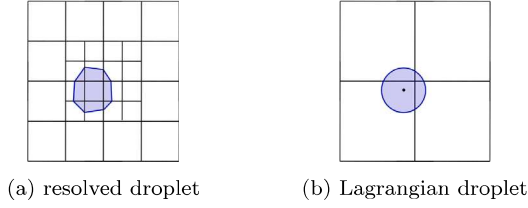


Fig. 3. Visualization of the grid cells in the vicinity of a droplet.

as in the present case. Per definition, $Oh = \frac{\mu_l}{\sqrt{\rho_l \sigma D_0}}$. For an accurate application of the Weber number criterion, we also ensure that the droplets remain sufficiently distant from the resolved liquid phase to accurately determine the undisturbed flow velocity. The quantity f_{density} defined in Section 2.4 is used for that. Moreover, we transfer droplets when they reach a certain distance from the coherent liquid jet surface to avoid regions with a high number of coalescence events. Transferring a droplet too soon, meaning it would have merged with another droplet at a later time, would increase the overall number of drops in the coupled formalism compared to pure Eulerian simulations and thereby reduce the mean diameter. To properly set the minimum distance from the coherent jet at which the droplets are transferred, we determine the location of coalescence and breakup events for pure DNS simulations with the help of the post-processing method described in Appendix C. This criterion is called “coalescence criteria” in the following. Finally, droplets in contact with the wall are not transferred.

The conversion of the resolved droplets to point-droplets is carried out in two stages. First, the volume fractions of liquid corresponding to the transferred droplet are set to 0. Then, the velocity of the gas medium (i.e. the cell values) is set to the undisturbed gas velocity in a spherical region at a distance $1.5 d_p$ from droplet centroid. We follow the suggestion of Ling et al. [18] and restore the undisturbed flow velocity field interpolating the velocity from the surface into the interior of a region centered at the particle location.

Droplet removal from VOF formalism is the key reason for saving computation time as there is no need for the fine cells to resolve their interface. Moreover, to reduce the amount of computation cells in case of DNS simulations coupled with the Lagrangian method, the maximum level of refinement for adaptation to velocity fluctuations was lowered by two levels compared to those of the liquid volume fraction. This is justified, as we do not aim to resolve the droplets inner flow patterns and the small-scale turbulent eddies of the gaseous phase, which are not affecting the droplet trajectories. Finally, the cells at the two highest levels are removed when transferring a resolved droplet to the Lagrangian framework (see Fig. 3).

2.3.3. Conversion back to resolved droplets

Should the droplets in the Lagrangian formalism approach the fluid phase again, as it happens for instance in the downwash region behind the jet, they will be resolved again. For illustration, the droplets trapped in the downstream recirculation with velocities opposite to the main air flow are shown with shades of blue in Fig. 4. The impact craters resulting from collision of those droplets with the leeward side of the jet surface are visible. Droplet proximity to the resolved interface is the only criterion for inverse conversion and is evaluated with f_{density} defined in Section 2.4. Lagrange-to-Euler transfer happens for $f_{\text{density}} > 0.05$ (for 5 percent of liquid in the rectangular region), when point-droplets are almost in contact with the resolved interface. This avoids the fact that droplets are transferred back immediately after being tracked in the Lagrangian solver. While the merging of Lagrangian droplets with the resolved interface is one reason for reverse Lagrange-to-Euler conversion, the expected breakup of a Lagrangian droplet would be another reason, as the Lagrangian method is free from breakup models. Criteria for determining fragmentation stability

can be applied to predict upcoming breakup events, which would be a combination of Weber number and aspect ratio. However, when the coalescence criterion for Euler-to-Lagrange conversion is used, Lagrangian droplets are generated away from the region with a high frequency of breakup events. The latter region includes the large recirculation. They will most probably stay away from that region, as the mean air velocity there is in the direction of the inflow velocity. The probability for further breakup is therefore very low. Moreover, the Weber number was already used as a local criterion for Euler-to-Lagrange conversion and the mean velocity of the air flow in relatively homogeneous in this region. The Weber number is not expected to increase so much. Therefore, criteria to assess droplet stability are not applied for reverse conversion.

Droplet reconstruction is achieved in 3 steps: first, the grid is refined in the region where the droplet is initialized with the diameter $d_p = (6V_p/\pi)^{1/3}$ up to the smallest level l such that, $\sqrt{3}\Delta(l) < d_p$ with $\Delta(l) = L_0/2^l$, then, the volume fractions are set according to the parameters of the transferred point-droplet.

In general, the volume of the resolved droplets initialized with the diameter of the point-droplet V_d is not equal to the volume of the equivalent sphere V_p , because restoring the shape parameters with Basilisk initialization function is more straightforward than the volume of the droplets directly. The difference is large as the refinement of the region that receives the droplet is coarse, only 1.7 to 3.4 cells per diameter are available. Therefore, in order to achieve mass conservation, the volume fractions in mixed cells are scaled by a correction factor (see Appendix A) in the last step. Refining the region up to the highest level of refinement would need a high computation effort, hence the method is a compromise between accuracy and computation time ensuring mass conservation. Taking the volume of a cuboid cut by a sphere would lead to the exact volume, but this would also be more time consuming. We note that Chéron et al. [20] use a minimization algorithm in droplet diameter to achieve mass conservation.

The velocity $\mathbf{u}'$ in the cells occupied by the resolved drop can be computed using the velocities of the point-droplets $\mathbf{u}_p$ and the previous velocity of the gaseous phase $\mathbf{u}$ in those cells (see [33]):

$$\mathbf{u}' = \mathbf{u} + \left(1 + \alpha \frac{\rho_g}{\rho_l}\right) (\mathbf{u}_p - \mathbf{u}) \quad (8)$$

with $\alpha = 0.5$ being the added-mass coefficient for a sphere. According to Ling et al. [18], as “a portion of the momentum of the droplet given in the conversion is transferred to the surrounding flow and used for the local perturbed flow development”, the momentum of the resolved drop is initialized not only with the momentum of the Lagrangian droplet, but the momentum of the perturbed flow is also added.

2.3.4. Two-way coupling

The Eulerian and Lagrangian solvers are two-way coupled via the source term in the Eulerian Navier–Stokes equation resulting from point-droplet’s change of momentum. Neglecting gravity and unsteady contributions, each point-droplet contribute to the momentum source with:

$$\Phi^p(\mathbf{x}) = \frac{\rho_l V_p \mathbf{a}_d}{(2\pi\sigma_p^2)^{3/2}} \exp\left(-\frac{(\mathbf{x} - \mathbf{x}_p)^2}{2\sigma_p^2}\right) \quad (9)$$

where droplets acceleration $\mathbf{a}_d$ during a given timestep is smoothed using a Gaussian distribution. The standard deviation σ_p is taken as the droplet diameter d_p in the present work, but other parameters for it can be found in the literature. S. Lomholt et al. [36] showed that for a Stokes flow and a two-way coupling force distributed with the standard deviation $r_p/\sqrt{\pi}$ the velocity field around the droplet is reproduced accurately for distances $r/r_d > 1.25$. G. Tomar et al. [17] take the maximum of the radius of the droplet and the size of the computational cell containing its center. Ling et al. [18] recommend a grid independent standard deviation between 5 and 10 times the

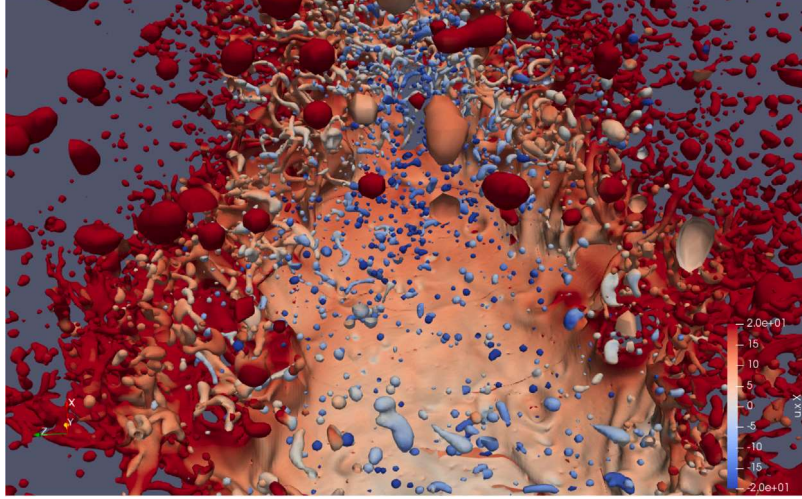


Fig. 4. Contour plot of the liquid surface at $f = 0.5$ with a view of the leeward side of the jet surface colored by the velocity component in air stream direction.

droplet diameter. However, the implemented value of $2d_p$ can be found in the source code Paris Simulator used by the authors. They concede that the distribution of the force achieves momentum conservation, but that the backward effect on the flow will only be captured at scales larger than the Gaussian broadening. The wake and the shear layer near the droplet interface will not be described. They refer to more sophisticated models to represent the perturbation in the flow [36,37]. Chéron et al. [20] give the expression for analytical discretization of the Gaussian smoothing kernel for a Cartesian uniform grid. We neglect inter-drop effects (4-way coupling), as we transfer droplets to the Lagrangian method far away from regions with a high density of coalescence events, hence also away from droplet-droplet aerodynamical interaction.

2.4. Parallelization of the Lagrangian solver

Each processor solves the equation of motion for a list of droplets whose centroids are located in local leaf cells. However, the region around Lagrangian droplets where the velocity of the undisturbed gas phase has to be set after removal of resolved droplets, or where the momentum source term is added to the acceleration in the Navier Stokes equations, could extend across several MPI domains for parallel runs (see Sections 2.4.1 and 2.4.2 for details of the implementation). Therefore, some processors have to know the information of specific droplets not included in their original list. To resolve this issue, it is helpful to define a minimal rectangular stencil around the droplets' centroid containing the cells where the field values have to be set. The list of droplets for a given processor has to be extended to include the droplets for which some of the leaf cells in the stencil are included in the processor domain.

Actually, field values are set in cells within the reach of a spherical region centered at the droplet's position, with a specific radius of either $1.5d_p$ or $3d_p$. The sought rectangular stencil is the smallest stencil including this spherical region. As visualized in Fig. 5, to define this stencil we follow the approach proposed by Tomar et al. [17]. First, we define the leaf cell containing the droplet's position. Subsequently, the smallest coarse cell including this leaf cell and satisfying the criterion that one of the cell-face is at a distance from droplet's position greater than the radius of the spherical region is identified. Finally, we determine all the equal-sized neighbors of the coarse cell intersecting the spherical region.

The knowledge of this rectangular stencil is also required for the evaluation of the droplet proximity to the dispersed liquid phase. The percentage of liquid phase in the rectangular stencil f_{density} is calculated for that, and is accessible with Basilisk octree grids without

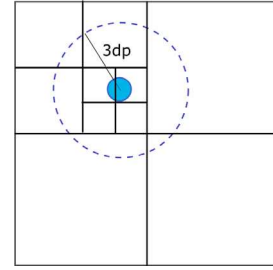


Fig. 5. 2D visualization of the rectangular stencil including a spherical region (dashed blue) around a droplet (filled with blue)

extension of the original list of droplets for a given processor. This is a criterion for transferring droplets. In the present work, droplets are transferred to the Lagrangian solver for $f_{\text{density}} < 10^{-4}$, and returned to DNS as resolved droplets for $f_{\text{density}} > 0.05$.

2.4.1. Update gas phase velocity after removal of resolved droplets

In this case, the spherical region is at a distance $1.5d_p$ from droplet centroid. For each cell in the droplet, the undisturbed velocity is interpolated from values in cells centers near 8 locations at a distance $1.5d_p$ from droplet centroid, as shown in Fig. 6. To find the corresponding cell centers we proceed as in Section 2.3.1.

2.4.2. The momentum source term

As the Lagrangian time step is large compared to the Eulerian one, we do not apply the momentum source term solely at the position of the point-droplet, instead it is distributed to the gas phase along the point-droplet trajectory in the last Lagrangian time step. The previous droplet position is shifted with the local flow velocity $\mathbf{u}_f$, where $\mathbf{u}_f$ is interpolated at the position of the droplet in the previous time step (see the explanations for Eq. (5)). We note that the cell size is $\Delta(10)$, as the adaptation to the velocity field is up to level 10 (Section 4.2.3). The momentum source is equally subdivided on positions on a line between droplet position at previous Lagrangian timestep t transported with flow velocity $\mathbf{u}_f$, and the current droplet position at $t + dt_{\text{Lag}}$. At each position, the momentum source is distributed using a Gaussian function assumed to vanish at a distance $3d_p$ from the location of its maximum value. The number of positions is chosen so that the Gaussian functions defined in Eq. (9) overlap (see Fig. 7). The processors involved are determined with the help of rectangular stencils including spherical regions of radius $3d_p$ centered at each position on the trajectory.

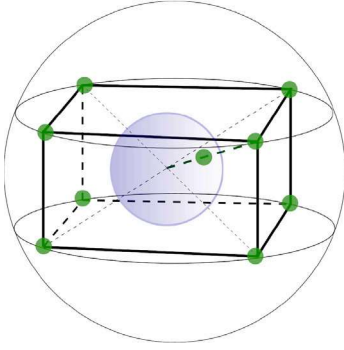


Fig. 6. Update gas velocity at position of the green dot inside the (blue) droplet: determine corners of a parallelepiped (marked with green dots) at a distance $1.5 d_p$ from the droplet centroid so that two corners are aligned with droplet centroid and the position where we want to interpolate.

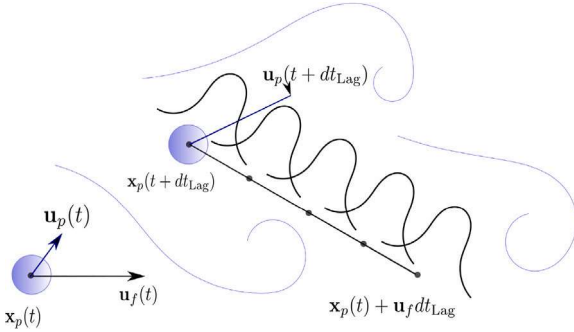


Fig. 7. Distribution of the momentum source term at $t + dt_{Lag}$ resulting from the trajectory of a given droplet visualized in blue for two successive Lagrangian time steps t and $t + dt_{Lag}$. Its location $\mathbf{x}_p$ and velocity $\mathbf{u}_p$ is indicated for both time steps. The line between the previous droplets position shifted with the local flow velocity $\mathbf{x}_p(t) + \mathbf{u}_f dt_{Lag}$ and the current droplet position $\mathbf{x}_p(t + dt_{Lag})$ is shown. The overlap between the Gaussian smoothing functions distributed on this line is shown.

3. Validation of DNS simulations

3.1. Setup

In this section, the atomization of Jet A-1 fuel in the jet in cross-flow configuration is investigated with DNS simulations. The setup is described, and a grid study is conducted. The standalone Eulerian simulations at the finest resolution able to reach the quasi-stationary state will serve as a reference and be compared with results from the coupled VOF and Lagrangian method Section 4.2.3.

3.1.1. Experimental configuration

The test conditions used for the simulations in the present work are defined by Rachner et al. [3] and are relevant to lean premixed prevaporized combustion in gas turbines. The experiments are conducted in a duct of rectangular cross section, which is 0.305 m long. The DNS focuses on a specific region of size $L_0 = 0.036$ m within the larger channel. The fuel injection orifice is located in the middle of the duct.

3.1.2. Computational domain

A cubic domain is considered (see Fig. 8).

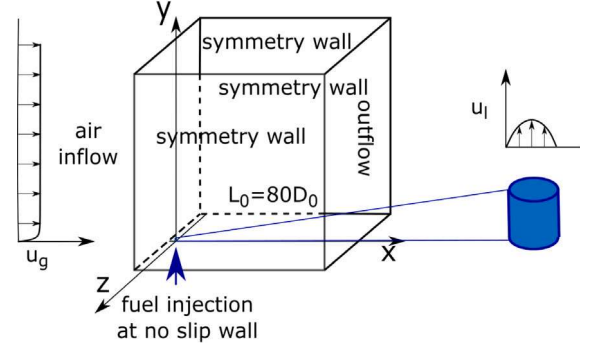


Fig. 8. Computation domain and initialization. The air inflow includes a boundary layer at the bottom wall (see Eq. (10)), and a parabolic profile is assumed for the liquid at fuel injection (Eq. (11)).

3.1.3. Boundary conditions and gas phase inflow conditions

The air inlet is located on the left-hand side of the computation domain and is the result of the flow through half the experimental channel. The air enters the channel with the constant velocity U_g . In fact, a turbulent boundary layer has developed, as the Reynolds number of the channel flow under consideration is $Re = \frac{\rho_g U_g L_0}{\mu_g} = 1.4 \times 10^6$, which is above the $Re = 4000$ threshold for which channel flows are typically turbulent. The investigation of the effect of turbulence at inflow is an interesting research topic, but out of the scope of the present work. Instead, we consider a laminar boundary layer given by the expression:

$$u = U_g \left(\frac{y}{\delta_x} \right)^{1/7} \quad (10)$$

At the position of the orifice, the boundary layer thickness is $\delta_0 = 2.5$ mm.

Symmetry boundary conditions (free-slip) prevail at the remaining side- and top walls, except at the bottom wall including jet inflow orifice, where Dirichlet (no-slip) boundary conditions are applied. The outflow boundary is implemented on the right-hand side of the cube, and the grid is coarsened for $x > 0.02925$ m to avoid backflow.

3.1.4. Liquid phase inflow conditions

As the injector is mounted flush in the experimental channel, it is reasonable to inject the fuel from a circular orifice at the bottom wall. The center of the orifice is located at a distance $X_0 = 0.001125$ m from the inflow boundary. We initialize the liquid phase as a cylinder with equal height and diameter $D_0 = 0.45$ mm. A parabolic velocity profile with mean velocity $\bar{u}_l$ is assumed:

$$u_l = 2\bar{u}_l \left(1 - \frac{x^2 + z^2}{(D_0/2)^2} \right) \quad (11)$$

The liquid jet Reynolds number $Re_l = \frac{\rho_l \bar{u}_l D_0}{\mu_l}$ is indicated in Table 1. The current focus is on the Lagrangian method for reducing computation time, therefore the turbulence in the liquid phase was not considered.

3.1.5. Operating conditions and material properties

The density and viscosity for kerosene Jet A-1 at $T = 20^\circ \text{C}$ are $\rho_l = 789.27 \text{ kg/m}^3$ and $\mu_l = 1.422 \times 10^{-3} \text{ kg/(m s)}$, respectively. Further, the surface tension is: $\sigma = 2.57 \times 10^{-2} \text{ N/m}$.

The operating conditions investigated in the present work are given in Table 1. The Froude number of the liquid phase $Fr = \bar{u}_l / \sqrt{g L_0}$ is larger than 16.7 (case U75q2). The effect of gravity compared to inertia force of the jet is therefore marginal and can be ignored (we follow the argumentation of Zhang et al. [38]).

According to the classification using the $We_g - q$ regime map proposed in the review paper of Broumand and Birouk [6], the jet

Table 1

Overview of the operating conditions for the baseline and U75q2 cases. q is the momentum flux ratio.

	Baseline	U75q2
U_g [m/s]	100	75
q [–]	6	2
p [bar]	5.8	5.9
$\bar{u}_l$ [m/s]	22.99	9.93
Re_l [–]	5745	2480
We_g [–]	1260	710
Oh [–]	0.015	0.015

primary breakup is located in the shear breakup (or sheet stripping) regime for the baseline case and in the mixed breakup regime for the U75q2 case. We note that Becker and Hassa [39] expected the column breakup mechanism to be predominant in the case U75q2, whereas the baseline case is surface breakup dominated. We take from the $Oh-We_g$ regime map, that the Ohnesorge number has no influence on the nature of the breakup.

3.2. Resolution

First, the turbulent length scales are estimated and compared with the size of the smallest computational cells, to evaluate the proportion of the energy spectrum we resolve in our simulations. We use Kolmogorov's theory to derive the smallest turbulent length scale of the gaseous phase, the Kolmogorov scale. We refer to the work of Garcia et al. [40] on the flow behind a long cylinder for a Reynolds number of $Re_g = \frac{\rho_g U_g D_0}{\mu_g} = 10^4$. The kinetic energy spectra show the $-5/3$ slope predicted by Kolmogorov's theory in the inertial subrange, followed by a rapid decay rate for the unresolved wave numbers. They estimate that the integral length scale is of the order of the diameter of the cylinder. Similarly, in the case of the flow behind a jet in crossflow, it is reasonable to specify the order of magnitude for the integral length scale as the diameter of the orifice D_0 .

The Kolmogorov scale η_g [41] is deduced from the Reynolds numbers Re_g with the diameter of the orifice $D_0 = 4.5 \times 10^{-4}$ m as the characteristic length. In this section, all the scales are evaluated for the baseline case, for which $Re_g = 18500$. For the case U75q2, all the scales are larger and easier to resolve.

$$\eta_g = \frac{D_0}{Re_g^{3/4}} = 2.8 \times 10^{-7} \text{ m} \quad (12)$$

The Taylor microscale is estimated as $\lambda_g = \sqrt{10} \eta_g^{2/3} D_0^{1/3} = 1.05 \times 10^{-5}$ m = $\mathcal{O}(10^{-5})$ m. It is impossible to resolve the smallest length scales with reachable computation time effort, as a mesh step $\Delta_l < 2\eta_g$ would be necessary for that. It is shown in Section 4.2.3, that the finest mesh for which the quasi-stationary state is reached corresponds to the maximum level of refinement 12 for adaption to the VOF variable. Turbulence is therefore resolved with cells of size $\Delta(12) = L_0/2^{12} = 8.8 \times 10^{-6}$ m = $\mathcal{O}(10^{-5})$ m for pure DNS simulations, and $\Delta(10) = L_0/2^{10} = 3.5 \times 10^{-5}$ m = $\mathcal{O}(10^{-5})$ m for coupled simulations, and both values are of the order of the Taylor microscale $\mathcal{O}(10^{-5})$ m and one order of magnitude lower than the integral length scale $\mathcal{O}(10^{-4})$ m. Hence, the energy containing eddies and part of the inertial subrange are captured by the simulations.

In the next step, the relaxation time of the point droplets tracked in the Lagrangian method τ_p is compared with the time scale of the turbulent eddies τ_f to see if the turbulence scales which influence droplet trajectories are resolved. The Stokes number is defined for that as:

$$Stk = \frac{\tau_p}{\tau_f} \quad (13)$$

In general, if the Stokes number is larger than one (large droplets), droplets do not see the eddy, whereas droplets with Stokes number $Stk \ll 1$ follow the flow closely. To obtain an estimate of τ_f , we can build the Stokes number with the integral time scale of turbulence $\tau_0 = D_0/U_g = 4.5 \times 10^{-6}$ s calculated with the velocity of the main flow $U_g = 100$ m/s. Further, when Re_p is small, i.e. if the droplet is almost adapted to the flow, $c_d = 24/Re_p$. Therefore, the expression for droplet relaxation time (see Eq. (6) in Section 2.2) reads:

$$\tau_p = \frac{\rho_l d_p^2}{18\mu_g} \quad (14)$$

In this approximation, the relaxation time of the smallest droplets transferred to the Lagrangian method with size $d_p = 2\Delta(12) = 1.8 \times 10^{-5}$ m is $\tau_p = 7.7 \times 10^{-4}$ s. Hence it comes out from this approximation that transferred droplets are not affected by turbulence eddies characterized by the integral time scale of turbulence τ_0 in the main flow, as $Stk \gg 1$ applies to these droplets.

However, we observe DNS droplets and Lagrangian droplets being captured by the recirculation (see Fig. 18), meaning $Stk \approx 1$, which can be explained as follows. On the one hand, the recirculation region downstream the liquid jet (Fig. 18) is characterized by $U_g \ll 100$ m/s and by turbulent coherent structures larger than the orifice diameter, which lead to a local time scale at least a factor 10 larger than τ_0 . On the other hand, for large relative velocities thus also large Re_p , $c_d = 24/Re_p$ is no longer valid. This leads to longer relaxation times than those calculated using Eq. (14). For example, for the smallest transferred droplets and $u_{rel} = 100$ m/s, $\tau_p = 5.3 \times 10^{-5}$ s can be calculated using Eq. (15) for the drag coefficient with $Re_p = 740$. Finally, we expect most of the turbulent scales which influence the Lagrangian droplets as being resolved.

The use of a fixed time step in the Lagrangian method is justified in the following. According to Bodnár et al. [42], and in the absence of droplet collision models, the Lagrangian time step should be adjusted considering the minimum of the particle response time, the integral time scale of turbulence and the time needed by a particle to cross a control volume. The fixed time step used in the present work $dt_{Lag} = 5 \times 10^{-6}$ s is of approximately the integral time scale of turbulence τ_0 for the baseline case calculated above, which is lower than the relaxation time of the smallest Lagrangian droplets $\tau_p = 7.7 \times 10^{-4}$ s and therefore imposes the Lagrangian time step used in the present work. Considering also the time needed for a particle to cross a control volume would lead to smaller Lagrangian time steps and significantly increase the computation time.

For illustration, the liquid surface including a close view on the coherent jet obtained with pure VOF simulations at the finest resolution is shown in Fig. 9 for both investigated cases. We note that, the error tolerance for adaption to both velocities and volume fractions are $\epsilon_u = \epsilon_f = 0.1$.

3.2.1. Droplet statistics

This section is concerned with quantitative validation. We investigate the sensitivity to mesh resolution of the droplet distributions and resulting Sauter Mean Diameter (SMD). These are the outcome of the simulations relevant for combustion applications. While DNS simulations of the liquid jet in crossflow atomization with the parameters of the present work are able to capture the liquid jet penetration depending on the large filaments and to resolve the instability waves on the jet column, they are generally not able to resolve the smallest length scales related to droplet size. In the following, the convergence behavior of the droplet size distribution is investigated. The latter is a good measure of the degree of convergence, as it covers all length scales related to the size of the liquid structures.

Only the baseline case defined in Table 1 is discussed in detail. Droplet size distributions of droplets collected in the whole computation domain are shown in Figs. 10 for the maximum levels of refinement 11 to 13. The simulations were carried out until the quasi-stationary

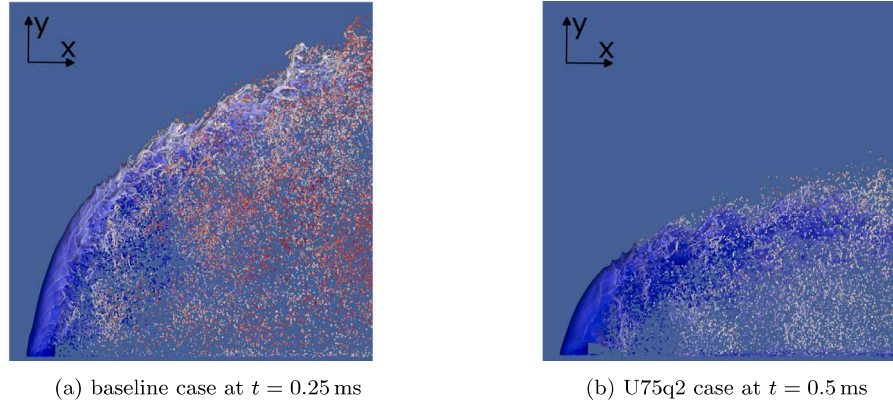


Fig. 9. Visualization of the fuel surface (PLIC) colored by the axial velocity for pure DNS simulations at level 12. The scale for the axial velocity runs from 0 (blue) to 100 m/s (red). Different views and time steps are available in the supplementary material.

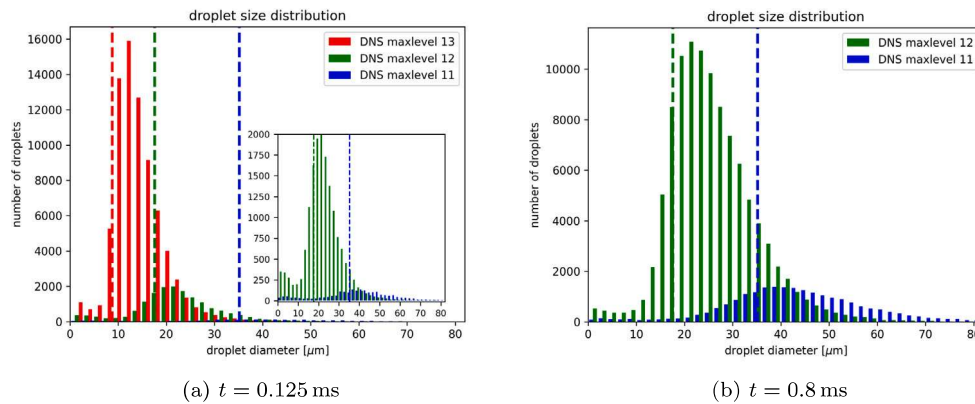


Fig. 10. Droplet size distributions for different resolutions and $x < 30$ mm (whole domain except the coarse region at outflow). The dashed lines indicate the cutoff droplet diameter, corresponding to twice the smallest cell size.

state was reached for the level of refinement 11 and 12. For level 13, we stopped at $t = 0.125$ ms due to the immense computing effort involved. This is why level 13 is missing in Figs. 10 (b). Vertical dashed lines indicate the cutoff droplet diameter, corresponding to twice the smallest cell size $\Delta(l)$. The corresponding smallest cell sizes are then: $\Delta(11) = 1.8 \times 10^{-5}$ m, $\Delta(12) = 8.8 \times 10^{-6}$ m, $\Delta(13) = 4.4 \times 10^{-6}$ m.

For all investigated time steps and levels of resolution, the number of droplets below this cutoff is always strongly enhanced at the next level of resolution. The simulation is unable to produce this under-resolved droplets, by separating them from existing structures. This threshold is also given by Pairetti et al. [43] in their work on the effect of mesh resolution on the atomization of a pulsating round liquid jet injected in quiescent air. Zhang et al. [44] remove them from their simulation (primary breakup of the so-called spray G.) and argue that, these under-resolved droplets could coalesce with larger liquid structures and prevent the distribution of the large droplets to converge, or falsify the size distribution the large droplets. They estimate the statistics of the missing droplets by fitting a log-normal distribution to the droplet distribution above the cutoff and by extrapolating this distribution towards the smallest droplets. Then, they deduce the percentage in terms of droplet mass below the cutoff and find out that they represent only a few percent. They claim that high-fidelity DNS can be viewed as detailed numerical simulations if the large-scale liquid structures are predicted accurately. This is the case when the distribution above the cutoff remains unchanged when the level of refinement is increased.

Actually, in the present case, the percentage of droplets in number and mass below the cutoff is very small and decreases with increasing

Table 2

Percentages of under-resolved droplets in the whole computation domain in terms of number and mass for different levels of refinement at the time $t = 0.125$ ms (a) and at the time $t = 0.8$ ms (b).

Level of refinement	11	12	13
% number	14.0	7.6	2.5
% mass	0.097	0.056	0.010
(a)			
Level of refinement	11	12	
% number	4.0	1.8	
% mass	0.044	0.011	
(b)			

resolution as shown in Table 2. The liquid volume contained in the under-resolved droplets that should be removed is very small.

However, the percentage of real physical droplets missing below the cutoff, which indicates how much liquid volume is still unpredicted by the simulation, is unknown. In our case, it is in general difficult to extrapolate the distribution to obtain the droplets smaller than the cutoff by fitting a log-normal distribution in the region corresponding to the droplets larger than the cutoff, as this region still changes with the resolution between level 12 and 13 in Fig. 10 (a). The detailed visualization of disintegration processes on the jet surface supports this observation. A qualitative comparison of the detailed jet surface in Fig. 11 between level 11 and 13, shows that level 11 fails to capture the correct topology of the instability waves close to the jet breakup.

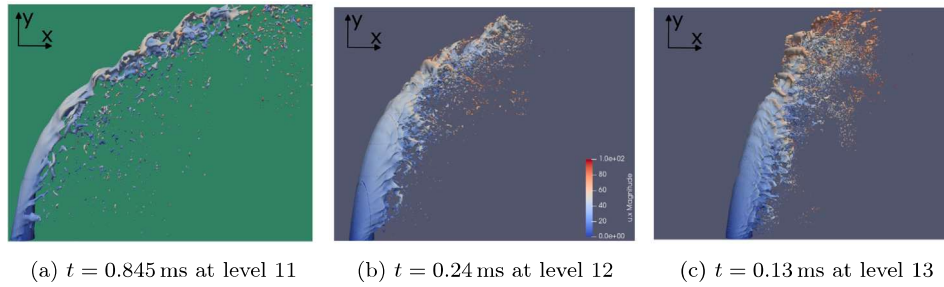


Fig. 11. Visualization of the jet surface (contour $f = 0.5$) for Jet A-1 fuel colored by the axial velocity. The scale for the axial velocity runs from 0 (blue) to 100 m/s (red). Simulations are performed with DNS only.

The rolling up of liquid at the crest of the waves due to counter rotating vortices originating from the baroclinic term in the vorticity equation [45] can already be seen at level 12, but the picture is more detailed at level 13. The rolled structures are better resolved, and lead to pearls when they detach from the jet. The separation of these structures from the coherent jet is the origin of the subsequent breakup processes. Therefore, the ability of the simulations to reproduce the correct distributions of the droplets larger than the cutoff at the later time and for a level of refinement of 12, will be related to the ability to capture the whole sequence of processes from primary to secondary breakup processes.

Figs. 12 and 13 display the droplet distribution for different space intervals in the direction of the air flow, which means at different distances from the jet for the early (Fig. 12) and later (Fig. 13) times displayed and for the different levels of refinement defined before. Droplets larger than the cutoff show a good convergence for the early time and for $x < 3$ mm in Fig. 12 (a), in particular, the distributions of droplets larger than 25 μm are identical between level 12 and 13, hence the extrapolation method proposed by Zhang et al. [44] could be applied there. In this case, the collected droplets result mainly from primary stripping process, as the breakup length is approximately $x_b \simeq 3$ mm for $t = 0.125$ ms (see Fig. 25). However, as the distance to injection increases, the difference in droplet distribution above the cutoff between level 12 and 13 becomes larger. Two reasons are given to explain this behavior: Firstly, secondary breakup produces less larger and more smaller droplets at the finer level 13, secondly, droplets are faster at the lower resolution (see Section 4.2.3) and therefore more droplets reach the region far away from injection at level 12. The same observation holds for Fig. 13, the difference in droplet distribution above the cutoff increases when the distance to fuel injection increases.

In summary, droplet distribution shows a good convergence in the range above the cutoff at level 12 at the early time and close to the jet injection. The breakup processes involved there is mainly the boundary layer stripping. Convergence becomes worse far away from injection, when the droplets result from the whole sequence of disintegration processes which have their origin in the column breakup. However, the part of the distribution above the cutoff for all droplets at the early time in Fig. 10 (a) shows an acceptable convergence at level 12, as this part of the distribution shows a much smaller difference between level 12 and level 13 than between level 11 and level 12 (see the insert in subfigure (a) of Fig. 10).

The SMD obtained by pure DNS simulations at level 12 are compared with those predicted by correlations found in the literature (see Table 3). Droplet sizes are ensemble averaged in the last third of the computation domain, where droplets are mostly stable against breakup. To take account for temporal fluctuations, droplets are collected for all time steps in the quasi-stationary regime, at which the list of droplets are registered. We note that these time steps are separated by 5×10^{-6} s. In the literature, different correlations for the SMD can be found. Becker and Hassa [39] offer far-field spray maps and correlations at $x = 80$ mm for a jet in crossflow under very similar operating conditions as those detailed in the present paper. Moreover, several correlations for

Table 3

Predicted SMD using different correlations.

SMD (μm)	Baseline	U75q2
simulations	32.0	37.0
Becker and Hassa [39]	29.3	33.6
Ingebo and Foster [47]	30.1	37.3
Song et al. [48]	31.3	44.0
Jasuja [49]	32.4	46.9

cross-current breakup are available in Lefebvre, McDonell, Atomization and sprays [46], in Tables 6.10 and 6.12. For the baseline case, the SMD obtained from our simulations at level 12 agrees well with the value predicted by the correlation of Jasuja, whereas the correlation of Ingebo and Foster is better suited for the case U75q2. For the baseline case, however, the latter predicts an SMD that is only 2 μm smaller than the value obtained from the simulations. At the same time, the SMD obtained from our simulations exceeds the values predicted by Becker and Hassa, whose test conditions are very similar to those considered here, by approximately 3 μm . Overall, the simulations overpredict the SMD by about 2–3 μm , which could likely be reduced by employing a higher spatial resolution, since the droplet size distributions are then expected to shift towards smaller droplet diameters. Even the part of the distribution corresponding to droplets larger than twice the smallest cell size may still change slightly. Such behavior was observed at early times, as explained above. However, it remains unclear to what extent the distribution would further evolve in the quasi-steady regime, since simulations at level 13 are computationally not affordable.

In summary, computations performed with a grid refinement level of 12 reproduce experimental measurements and correlations used by jet-engine injector manufacturers for the SMD with an accuracy of approximately 2–3 μm . This level of accuracy is considered acceptable for generating spray boundary conditions for large-scale Eulerian–Lagrangian combustion chamber simulations.

It is also interesting to compare the SMD as a function of the distance from the bottom wall resulting from simulations in Fig. 14 (upper subfigures) with the experiments of Becker and Hassa [39]. Simulation results for single time steps at the border of the quasi-stationary regime are also displayed. In the experiments, all droplets crossing a registration plane located at $x = 80$ mm are collected. The experimental profiles correspond to a larger distance downstream from the point of injection than those obtained from simulations, which results in a deeper penetration of the spray plume. In order to compare the SMD profiles, the distance to the bottom wall on the horizontal axis is normalized with the maximal penetration. Despite this difference in the droplet registration, we observe a good agreement between simulations and experiments regarding the minimum and maximum values of the SMD and for both investigated cases. For the baseline case, however, the SMD curves exhibit opposite changes in concavity at the inflection point, which is probably due to analysis location. It can be observed, that the large droplets can be found in the upper part of the spray plume for both investigated cases, however in the case U75q2,

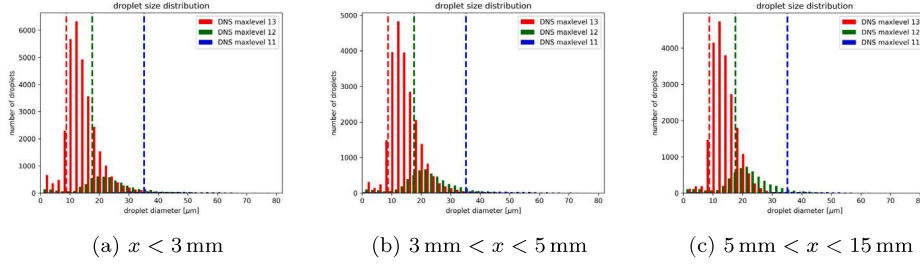


Fig. 12. Droplet size distributions for different resolutions at $t = 0.125$ ms. The limits of the intervals are indicated in Fig. 14 (bottom left). The dashed lines indicate the cutoff droplet diameter, corresponding to twice the smallest cell size.

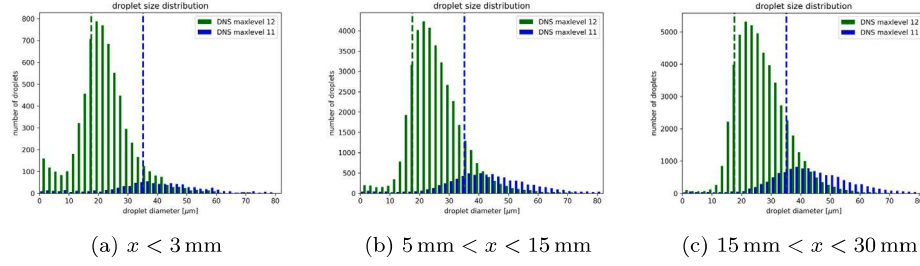


Fig. 13. Droplet size distributions for different resolutions at $t = 0.8$ ms. The dashed lines indicate the cutoff droplet diameter, corresponding to twice the smallest cell size.

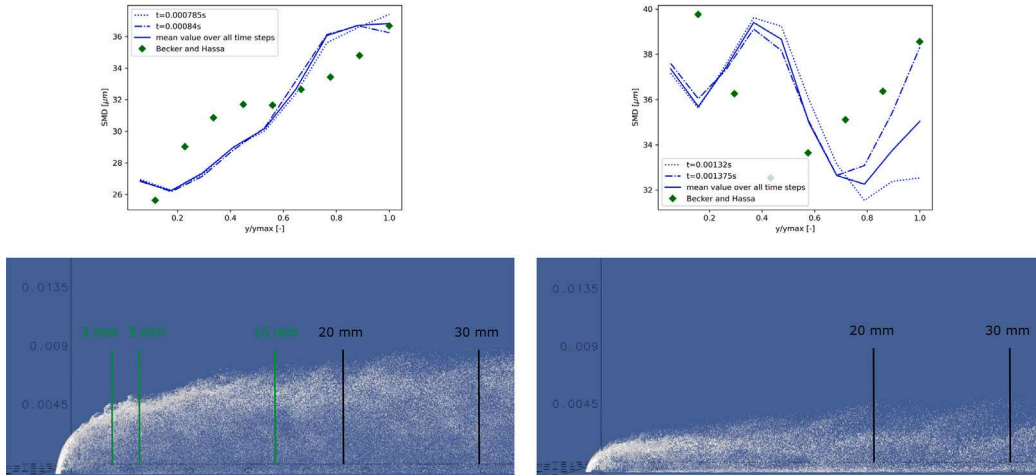


Fig. 14. Profiles of SMD versus distance from bottom of duct with droplets collected between $x = 20$ mm and $x = 30$ mm for the baseline case (subfigures on the left) and the U75q2 case (subfigures on the right). The results are displayed for two different time steps at the border of the quasi-stationary regime and for all the Lagrangian time steps in the quasi-stationary regime. For comparison, the experimental results by Becker and Hassa [39] are superimposed. The distance y from bottom of duct is normalized with the maximum value of jet penetration. Snapshots of the whole spray in the quasi-stationary regime state are shown for both cases (figures on the bottom). The limits of the interval for which droplets are collected are indicated with black lines.

large droplets are also located in central part of the spray plume as shown qualitatively in the snapshots in Fig. 14 (lower subfigures). We note that the large droplets near the lower wall are not measured in the experiments for the case U75q2.

4. Verification and validation of the Lagrangian method

4.1. Visualization of droplets trajectories

In this section, the positions of the Lagrangian point-droplets are compared qualitatively with those of the equivalent resolved droplets obtained from pure DNS simulations. In Fig. 15, the concerned droplets can be observed at the beginning of the atomization for the selected case U75q2. We note that the refinement is the same for pure DNS and DNS coupled with the Lagrangian solver (10 for the velocity field,

and 12 for the VOF field). Due to that, and at this early stage of the atomization process, the behavior of the resolved liquid phase is very similar for both methods. The position of the resolved droplets in the pure DNS can be mapped with the corresponding position of the Lagrangian point-droplets from the DNS coupled with the Lagrangian solver solution. The focus is on the top view of the upper part of the jet in crossflow atomization process and two different snapshots separated by the Lagrangian timestep are chosen: timesteps $t = 4 \times 10^{-5}$ s and $t = 4.5 \times 10^{-5}$ s. In every subfigure, the cells filled with a liquid volume fraction above a threshold value $f > 10^{-4}$ are represented. This threshold value is used by the tag function to identify the coherent liquid structure (see Section 2.3.1). Therefore, each cluster of neighboring colored cells corresponds to a resolved drop identified by the tag function. The figures on the left-hand side display results from coupled simulations, Lagrangian point-droplets (multicolored spheres), as well

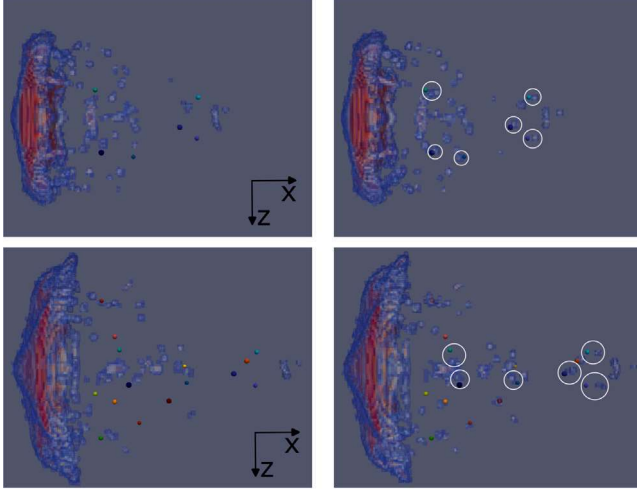


Fig. 15. For the case U75q2, top view with $y > 0.003\text{m}$ of the cells (no PLIC resolved interface) colored by the volume fraction of liquid $f > 10^{-4}$ (the colors evolve from blue for $f = 0$ to red $f = 1$) for DNS coupled with the Lagrangian method (left Figures) and for pure DNS, where the Lagrangian droplets from the coupled run have also been superimposed (right Figures). The top figures are taken at $t = 4 \times 10^{-5}\text{s}$, the figures below at $t = 4.5 \times 10^{-5}\text{s}$. The Lagrangian droplets are represented by equal sized multicolored spheres, and they keep their color between both timesteps. Encircled are the point-droplets already present at $t = 4 \times 10^{-5}\text{s}$, together with their corresponding resolved droplets.

as liquid structures resolved by the DNS. Results from pure DNS (i.e. no coupling with Lagrangian solver) are shown on the right-hand side. Here, for sake of comparison, Lagrangian point-droplets, which were obtained from the coupled simulations are superimposed to the DNS results. It can be observed that the Lagrangian droplets, which have been superimposed afterwards, follow very closely the trajectories of the next droplets resolved with pure DNS simulation (encircled together for all the point-droplets already present at $t = 4 \times 10^{-5}\text{s}$), with however, a slight delay with respect to the corresponding resolved droplet.

4.2. Quantitative verification and validation

4.2.1. Single droplets

We consider first a single resolved droplet of size $D_0 = 30\text{ }\mu\text{m}$ initialized with velocity components in the x and the y directions, $u_x^0 = 90\text{ m/s}$ and $u_y^0 = 20\text{ m/s}$, respectively. The size of the cubic computational domain is $L_0 = 2.4\text{ mm}$. There is a constant and homogeneous gas inflow at the left boundary with velocity $U_g = 100\text{ m/s}$ in x -direction. The droplet position and velocity as a function of time are shown in Fig. 16. Both, the results obtained from DNS and those obtained when coupling the Lagrangian solver to the DNS are displayed. For adaption at each timestep, four different maximum levels of refinement L_n between 8 and 11 are considered, but the region where the droplet is initially constructed is refined up to level 11 for all cases. We note that for level 8, the minimum cell size is $\Delta(L_8) = L_0/2^8 = 9.4\text{ }\mu\text{m}$, which is approximately the smallest cell size of our reference simulations of $\Delta(L_{12}) = 8.8\text{ }\mu\text{m}$. For coupled simulations, the droplet is tracked with DNS only at the beginning of the simulations. Then, after a Lagrangian timestep $dt_{\text{Lag}} = 5 \times 10^{-6}\text{s}$, the droplet is transferred to the Lagrangian solver. As can be seen in Fig. 16 (a,b), the trajectories are very similar for all cases, which shows that the droplets are transferred properly. Differences between DNS and Lagrange can be observed when analyzing the velocity components in Fig. 16 (c,d), however these diminish with increasing resolution as shown in Table 4. At level 8, the velocity component in direction of the air flow differ by 1.25 percent for a traveled distance of 2 mm, and the position by 0.75 percent in

Table 4

Validation of a single droplet with constant air inflow (see Fig. 16): deviation in percent of the velocity components u_x (a) and u_y (b) obtained with the VOF method compared to the results with Lagrangian tracking.

Level of refinement	8	9	10	11
% u_x	1.26	0.58	0.44	0.15
(a)				
Level of refinement	8	9	10	11
% u_y	14.42	6.45	4.61	1.95
(b)				

this direction. Therefore, for the whole length of the domain of 30 mm, the difference in position and velocity is of the order of 10 percent for droplets resolved with three cells per diameter. Furthermore, the slope of the time dependent velocity components for droplets resolved with the VOF method, corresponding to the acceleration, tend towards the slope for Lagrangian point-droplets with increasing resolution. The fact that the acceleration for Lagrangian droplets depends very little on resolution is comprehensible, as the velocity field remains mainly constant and homogeneous in the small computation domain. The drag force modeling under the assumption of quasi-steady forces is expected to be a good approximation here. This is confirmed by the agreement with the results from well-resolved DNS regarding the acceleration. For poorly resolved DNS droplets, however, the trajectory of the droplets is less accurate. The acceleration is larger and the droplets therefore move faster in direction of the air flow.

As Re_p varies between 1848 and 1100, the correlations used for the drag coefficient with $w = \log_{10}(Re_p)$ are mentioned in Eqs. (15) and (16):

$$c_d = \exp(3.78430 - 2.58857w + 0.35874w^2), \quad \text{for } 259.7889 < Re_p < 1526.087 \quad (15)$$

$$c_d = \exp(-5.65768 + 5.88495w - 2.14025w^2 + 0.24154w^3), \quad \text{for } 1526.087 < Re_p < 1.200229 \times 10^4 \quad (16)$$

4.2.2. Location of coalescence and breakup events from pure VOF simulations

Coalescence events occur mainly in the downwash region close to the jet, as illustrated in Fig. 17 for the baseline case. The post-processing method to identify coalescence and breakup events is described in Appendix C. This region with a large number of coalescence events is defined by complex recirculation patterns behind the jet, as can be seen in Fig. 18. The location of droplet break up events are shown in Fig. 19.

The size distributions of the droplets involved in coalescence and breakup processes are shown in Fig. 20. As expected, the distribution shifts to the right, i.e. towards bigger droplets as they merge (see Fig. 20 (a)). On the contrary, the distribution shifts to the left, i.e. towards smaller droplets as they undergo secondary breakup (see Fig. 20 (b)). Noteworthy the fact that coalescence and breakup processes approximately balance each other out in terms of droplet distributions. Also, we notice that some merged liquid structures have only a corner or an edge in common. These merged droplets are then identified as single droplets, but quickly separate again, which partly explains the compensation.

4.2.3. Droplets total count and distribution

The detailed interpretation of the results shown in the present section is given for the baseline case without and with application of the coalescence criterion. The results for case U75q2 are similar

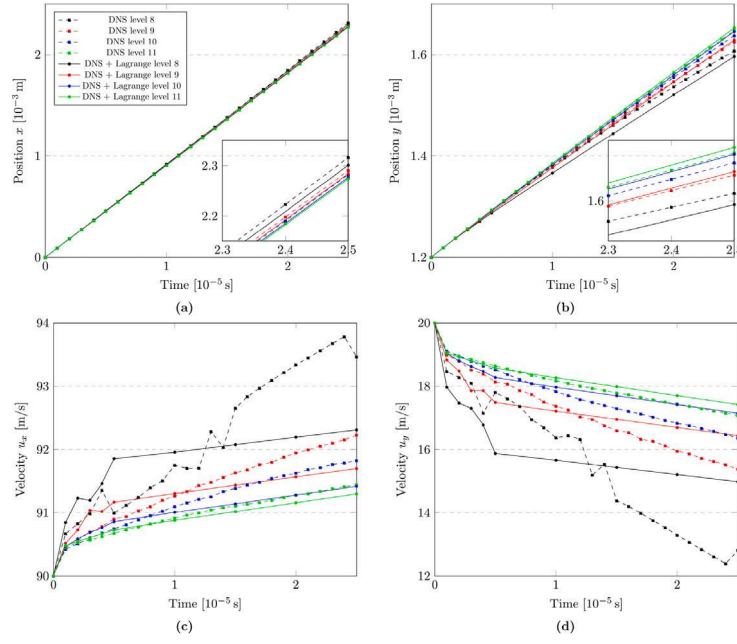


Fig. 16. Trajectory of a single droplet at different resolutions in a homogeneous and constant gas flow. Droplet position ((a) and (b)) and velocity ((c) and (d)) components are shown. Droplet initialization up to the maximum level of refinement of 11 is the same for all cases. Dashed lines correspond to results from simulations with DNS only, and solid lines to results from DNS coupled with the Lagrangian method with the timestep dt_{lag} and the velocity field refined up to level $L_n - 2$ only.

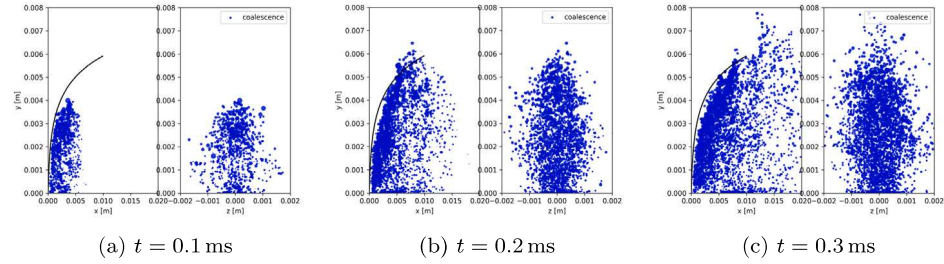


Fig. 17. Location of coalescence events at different timesteps.

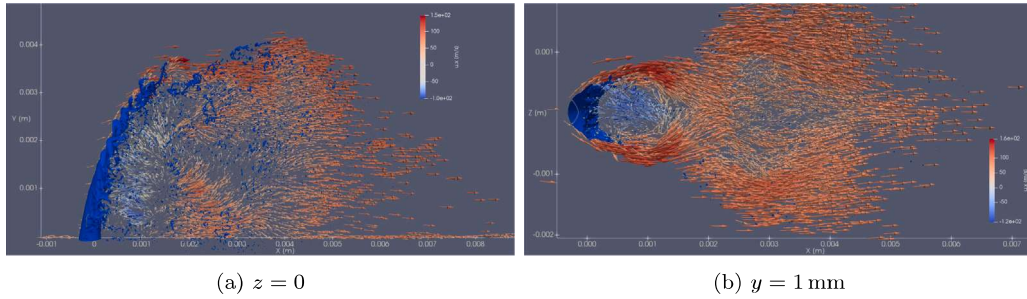


Fig. 18. Velocity field for VOF simulations of the baseline case at $t = 0.1$ ms in different regions. The level of refinement is 12. The velocity arrows are oriented and scaled by the velocity magnitude and colored by the axial velocity. The jet contour is shown in dark blue.

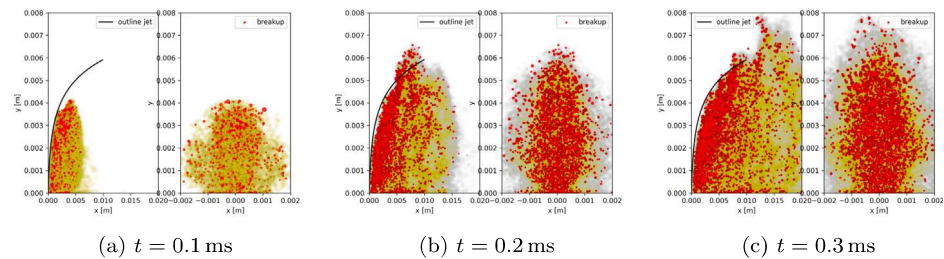


Fig. 19. Location of secondary breakup events (red dots) at different timesteps. The location of the whole droplets are indicated in green and gray.

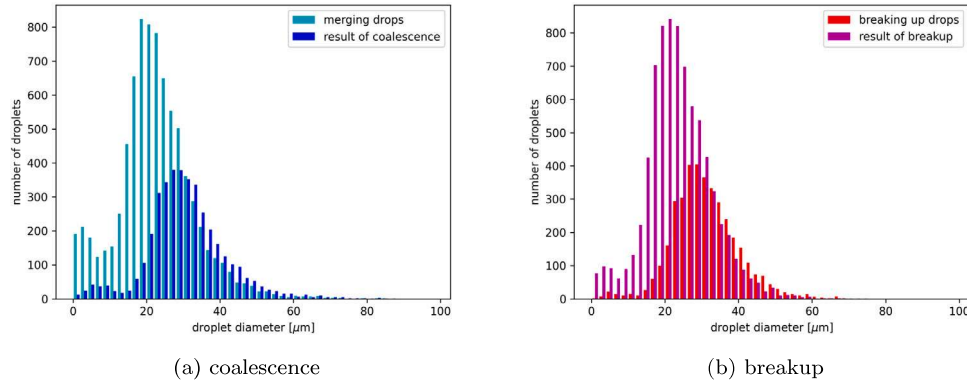


Fig. 20. Size distributions of the droplets involved in coalescence and breakup processes. For each process, the distributions of droplets prior to and after the event are shown.

and summarized at the end of this section for the sake of completeness. In this section, the maximum level of refinement is 12, except for the velocity field in case of coupled simulations (level 10). To further validate the coupling, the timewise evolution of total number of droplets within the computational domain is plotted in Fig. 21 (a) (solid curves). We note that the slope of the total number of droplets as function of time decreases significantly when droplets begin to leave the computation domain at the outflow. Results from pure DNS simulations are compared to the results of coupled solver computations. The droplet size distributions (Fig. 21 (b–e)) are compared. The main outcome is that the results from pure DNS and coupled Euler–Lagrange simulations fit quite well together when the coalescence criterion is applied regarding total number of droplets (solid blue and green line in Fig. 21 (a)) and droplet size distribution (Fig. 21 (d)) until droplets begin to leave the domain.

Without application of the coalescence criterion, an excess of overall number of droplets is observed in the coupled computation compared to pure DNS simulations (solid orange curve in Fig. 21 (a)). As the main process is a disintegration of the liquid jet in small droplets due to aerodynamic forces, droplet stability with regard to breakup is ensured using the Weber number criterion. The liquid phase is very dilute in the gaseous phase, hence the number of droplets undergoing coalescence can be considered low to a first approximation. However, coalescence processes were identified as the main reason for the large number of droplets in the coupled simulation with respect to the pure DNS simulation (see Appendix B). Actually, after the droplets are ejected from the liquid jet and for those trapped in the recirculation region downstream of the jet, there is a non-negligible probability of colliding with other droplets and merging, i.e. coalescence. The phenomena is only captured in the pure DNS case and leads to a reduction in the total number of droplets, as opposed to the droplets transferred to the Lagrangian solver, which does not have a coalescence model. In fact, a few merging droplets were first visualized at the beginning of the atomization for a small number of droplets in Fig. C.32, and then identified in a systematic way for a large number of droplets via post-processing at more advanced times, as shown in the previous Section 4.2.2.

Other potential reasons for the difference in total number of droplets between pure VOF simulations and those coupled with the Lagrangian method as detailed in Appendix B are less important and discussed in the following. For both investigated cases, a slight difference in droplets numbers provided by the atomization is expected due to the coarser resolution of the velocity field in the bulk phases (two levels smaller). The source term in the Navier–Stokes equations coming from the effect of Lagrangian droplets is expected to influence the disintegration to a small extent, as the conversion of the droplets takes place mainly downstream from the atomization process.

Therefore, a new criterion which accounts for the region with high coalescence density was applied: only droplets located at least

a distance of 6 mm away from the coherent jet are transferred. This is an empirical value valid for the 2 cases investigated here. Most coalescence events have then occurred prior to the transfer. This led to a reduced total number of droplets in coupled simulations, which was very close to the values from pure DNS simulations. The supplementary number of droplets still observed for coupled simulations at later time when droplets begin to leave at outflow can be explained by the lower velocity of the droplets in coupled simulations compared to pure VOF simulations. As mentioned in Appendix B, the number of droplets leaving at outflow is one the reason for the difference in total number of droplets between pure DNS simulations and coupled simulations. Poorly resolved droplets in pure DNS simulations are faster in direction of the main air flow than the point-droplets in the Lagrangian method. This was observed in the single droplet validation in Section 4.2.1.

We apply the same conversion criteria including the one concerning the coalescence to the second case, U75q2, and achieve good agreement between the pure DNS simulations and those coupled with the Lagrangian method regarding the total number of droplets as well as droplet size and velocity distributions (Figs. 22). Summarizing, the issue of the excess number of droplets for coupled simulations resulting from coalescence events has been addressed by introducing a lag in the transfer to the Lagrangian solver to account for coalescence events.

4.2.4. Jet penetration and column breakup point

In this section, spatial droplet distribution in the XY-plane is investigated in Fig. 23. The sum of all droplets in Z-direction is displayed. Correlations for jet penetration are also represented. The simulations accurately predict the jet penetration with DNS simulations for a maximum of 12 levels of refinement, and this is also the case when coupled to the Lagrangian method. Droplets spreading in the ZY-plane is also similar for pure Eulerian and Euler–Lagrange simulations (see the histograms in Fig. 24). Finally, the position of the column breakup point is not altered by the coarser resolution of the velocity field when VOF simulations are coupled to the Lagrangian method. As can be seen in Fig. 25, the breakup distance and height over time is very similar. Summarizing, a quantitative comparison of jet-penetration depth and column-breakup location between pure DNS and the combined DNS-plus-Lagrangian approach confirms the validity of the Lagrangian solver.

4.3. Computational cost

The simulations were performed at the SUPERMUC-NG at Leibniz Supercomputing Centre in Munich on 1152 CPU cores. The real computation time of 16 days were needed to reach to quasi-stationary state in the case of pure VOF simulations for the baseline case. We show the gain in computation effort obtained by coupling DNS with the Lagrangian method compared with pure DNS simulations. DNS

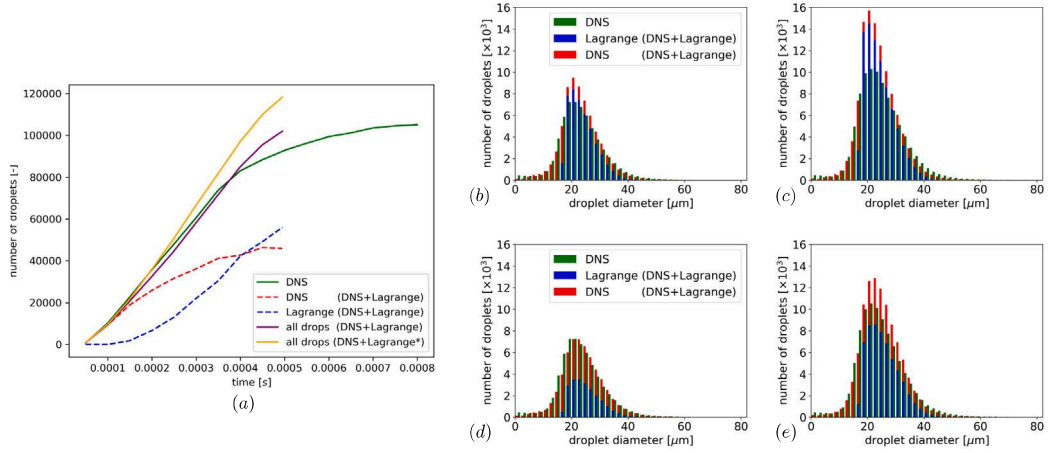


Fig. 21. Comparison of the total number of droplets for DNS (green) and DNS coupled to Lagrange (purple) for the baseline case (a). For coupled simulations, we distinguish between the resolved droplets (dashed red curve) and the point-droplets (dashed blue curve). The orange curve shows the total number of droplets without using the coalescence criterion. Comparison of droplet size distributions for DNS and DNS coupled to Lagrange for the baseline case: original simulations at $t = 0.3$ ms (b), and $t = 0.495$ ms, (c), simulations with the coalescence criterion at $t = 0.3$ ms (d), and $t = 0.5$ ms (e). The red DNS bars are added on the top of the blue Lagrange bars so that the top of the red bar shows Lagrange + DNS drops.

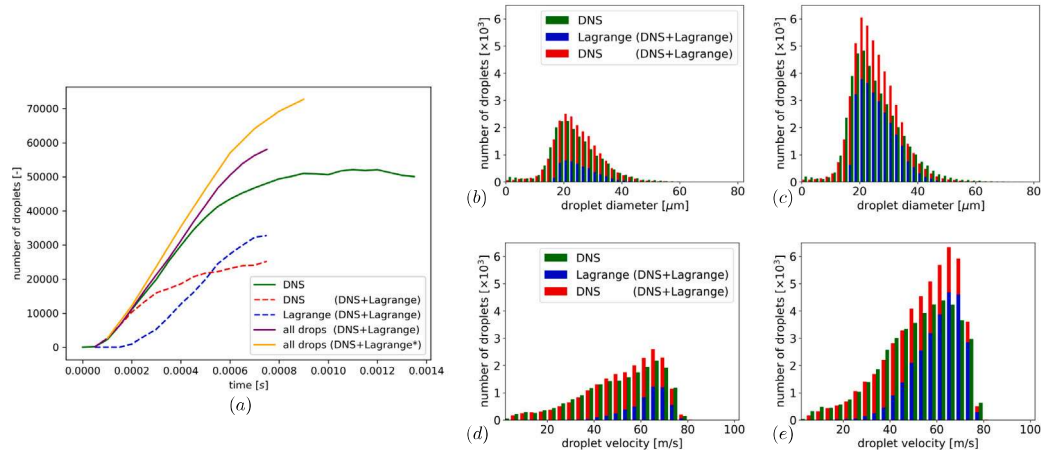


Fig. 22. Comparison of the total number of droplets for DNS (green) and DNS coupled to Lagrange (purple) for the case U75q2 (a). For coupled simulations, we distinguish between the resolved droplets (dashed red curve) and the point-droplets (dashed blue curve). The orange curve shows the total number of droplets without using the coalescence criterion. Comparison of droplet size distributions for DNS and DNS coupled to Lagrange with the coalescence criterion: droplet size distributions at $t = 0.3$ ms (b), and at $t = 0.6$ ms, (c), droplet velocity distributions at $t = 0.3$ ms and at (d), $t = 0.6$ ms (e).

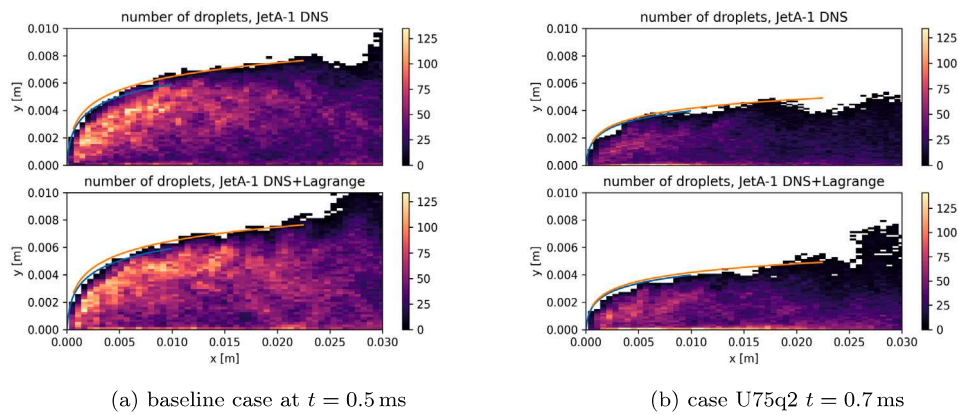


Fig. 23. Comparison of droplets histograms in the XY-plane for DNS and DNS coupled to Lagrange. Correlations for near-field penetration according to Becker and Hassa [39] (blue line), and Freitag, Hassa [50] (orange line) are shown.

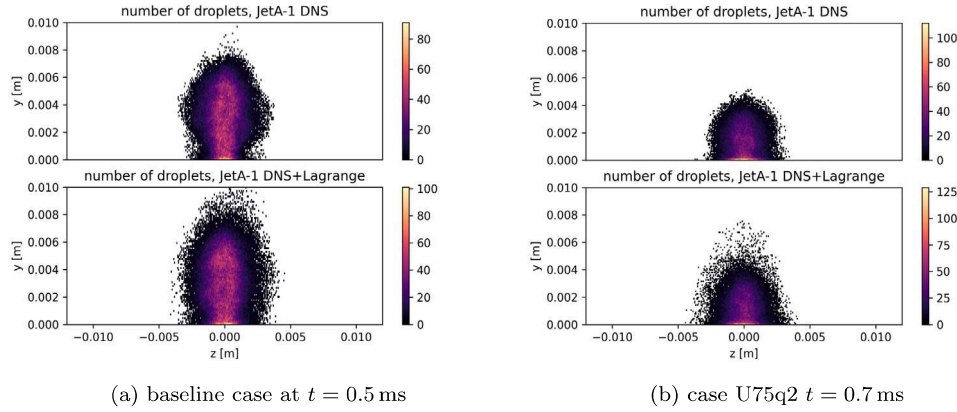


Fig. 24. Comparison of droplets histograms in the ZY-plane for DNS and DNS coupled to Lagrange.

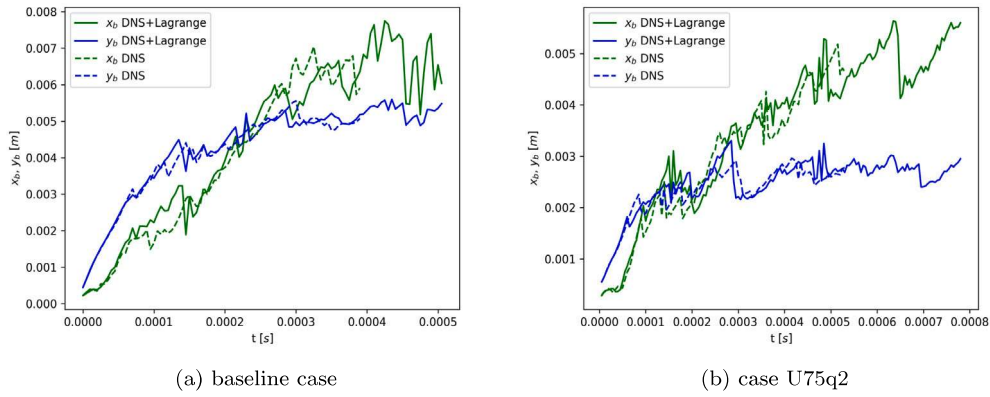


Fig. 25. Comparison of the column breakup distance x_b and height y_b between pure DNS simulations and coupled simulations for the investigated cases.

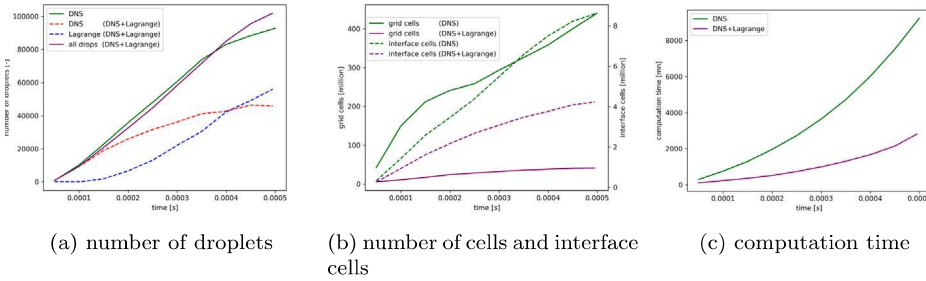


Fig. 26. Comparison of the computation effort in the baseline case between pure DNS and the coupled DNS and Lagrangian method.

simulations are performed with a maximum of 12 levels of refinement for adaptation to spatial fluctuations of velocity and liquid volume fractions. In order to save computation time, we transfer a major part of the droplets to the Lagrangian framework. Removal of resolved droplets lead to the reduction of the number of grid cells, so that the computation time decreases. As most of the grid cells are required to resolve the fluctuation of the gas phase velocities in DNS simulations, computation time is further reduced by decreasing the resolution in the gas phase. This choice is discussed in Section 3.2. To that purpose, the maximum level of refinement for adaptation to velocity fluctuations is set to the value 10. The time evolution of the number of droplets, computation cells and interface cells (for which the liquid/gas interface is reconstructed), as well as the computation time is shown in Figs. 26. Computation time was significantly reduced by a factor of about 3.5 by coupling DNS to the Lagrangian method. It is noteworthy that beside the savings in computation time also the accuracy can be improved by properly modeling poorly resolved liquid structures.

5. Conclusion and outlook

In this paper, a multi-scale simulation approach is applied to the atomization of a plain liquid jet in crossflow. The liquid-gas interface (jet and large ligaments) is accurately captured using the Basilisk Volume-of-Fluid method. We take advantage of octree adaptive mesh refinement, which reduces the computational effort significantly. An post-processing algorithm able to localize the coalescence events between resolved droplets was developed. Therefore, droplet conversion criteria could be defined, allowing to transfer the resolved droplets which are stable against breakup and coalescence to the LPP formalism. Both solvers are coupled via momentum coupling and two-way droplet conversion. In the case of coupled VOF and Lagrangian simulations, a coarser smallest cell size is used for adaptation to spatial velocity variations than to those of the VOF variable. This greatly reduces the amount of computational cells when droplets are removed from the DNS treatment.

First, we investigated the convergence of simulations with the VOF method alone. At the resolution used in the present work, allowing to reach the quasi-stationary state for the cases investigated, convergence is achieved concerning jet penetration. Concerning droplet size distributions, a shift is observed to smaller droplets at the next higher level of resolution. This fact is qualitatively confirmed by the observation of the jet surface. Finer structures are observed, for example the rolling up at the crest of the jet instabilities. However, good agreements with correlations from experiments are found regarding the Sauter Mean Diameter and jet penetration.

Then, the Lagrangian method implemented was validated quantitatively and qualitatively for single droplets. The validation of single droplets in a constant air flow shows that Lagrangian trajectories are more accurate than those of poorly resolved droplets within the VOF method. The global visualization of the trajectories of the transferred droplets at the beginning of the atomization process shows a very good match. At early simulation times, we obtained very similar number of droplets from coupled simulations as for pure VOF simulations, and droplet size and velocity distributions were in good accordance. However, at later simulation times, coupled simulations provide more droplets, which is partly due to the smaller mean droplet velocity. The discrepancy is observed when the first resolved droplets start to leave the computation domain. Computational time was reduced by a factor of about 3.5 by coupling the Lagrangian to the VOF method and by using a coarser resolution of the velocity field. Time savings are mainly due to a larger Lagrangian timestep and coarser adaptation to velocity fluctuations than to liquid volume fraction.

In future work, the effect of turbulence at inflow of both the liquid and gaseous phase have to be investigated. Subgrid-scale modeling can be included in momentum and mass conservation equations, which could change the topology of the primary and secondary breakup. It would also be beneficial to transfer more droplets to the Lagrangian method including breakup and coalescence models, in order to reduce the computation effort further, while maintaining accuracy.

CRediT authorship contribution statement

C. Kieffer-Roth: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation. **P. Le Clercq:** Writing – review & editing, Validation, Supervision, Investigation, Formal analysis, Conceptualization. **J.A. van Hooft:** Writing – review & editing, Software. **G. Eckel:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Transferring a Lagrangian droplet back to a DNS droplet

In general, three contributions to the volume of the reconstructed droplet V_d can be defined, with f_i^d (i the list of cell indices) the volume fractions:

$$\begin{aligned} V_d &= V_d^{cor} + V_d^1 + V_d^> \\ &= \sum_{f_i^d < 1, f_i^d + f_i \leq 1} f_i^d dV_i \\ &\quad + \sum_{f_i^d = 1, f_i^d + f_i \leq 1} f_i^d dV_i + \sum_{f_i^d + f_i > 1} f_i^d dV_i \end{aligned}$$

In order to explain the different terms, we note that the cells involved in the initialization of the reconstructed droplet may already be filled with a liquid volume fraction $f_i > 0$. Latter cells would be overfilled when the total volume fraction is greater than 1, i.e. $f_i + f_i^d > 1$. If this is the case, they contribute to the volume $V_d^>$. On the contrary, the cells for which $f_i^d < 1$ contributing to the volume V_d^{cor} , and those for which $f_i^d = 1$ included in V_d^1 do not lead to overfilled cells. In the following, we give the procedure for correcting the volume fractions of the reconstructed droplet f_i^d , so that the volume of the point-droplet V_p is recovered. This procedure is detailed for the general case, where overfilled cells are present. When the reconstructed droplet is far from the existing resolved interface, there are no overfilled cells and the equations simplify: The volume contributions $V_d^>$ and V_d^{1-f} can be removed. Both configurations, without and with overfilled cells, are displayed in Figs. A.27–A.29. In all the figures, the sub-figures on the left and on the right are respectively without and with overfilling. The red line indicates the position of the interface of the reconstructed droplet before correction (f_i^d). The volume fractions of the reconstructed droplet after correction is visualized in green, whereas the color blue indicates the liquid phase already tracked by the VOF method (f_i).

A.1. Over-estimated droplet volume

Most of the time, droplet volume is over-estimated after reconstruction with Basilisk initialization function. This means that the volume of the reconstructed droplet is larger than the volume of the original point-droplet: $V_d > V_p$.

- Case A: If the condition $V_p > V_d^1 + V_d^{1-f}$ holds, the reconstructed volume fraction in all interface cells $f_i^d < 1$ is scaled with the same multiplicative factor $\alpha < 1$, filled cells are unchanged, and $f_i^d = 1 - f_i$ is set in overfilled cells (see Fig. A.27).

$$\begin{aligned} V_p &= \alpha \sum_{f_i^d < 1, f_i^d + f_i \leq 1} f_i^d dV_i \\ &\quad + \sum_{f_i^d = 1, f_i^d + f_i \leq 1} f_i^d dV_i + \sum_{f_i^d + f_i > 1} (1 - f_i) dV_i \\ V_p &= \alpha V_d^{cor} + V_d^1 + V_d^{1-f} \end{aligned}$$

Combining the expressions for V_p and V_d , the correction factor reads:

$$\alpha = \frac{V_p - V_d^1 - V_d^{1-f}}{V_d - V_d^1 - V_d^>} \quad (\text{A.1})$$

- Case B: However, if $V_p < V_d^1 + V_d^{1-f}$ (see Fig. A.28), full cells are scaled to obtain the desired volume V_p , whereas the cells $f_i^d < 1$, $f_i^d + f_i \leq 1$ making up V_d^{cor} are set to zero, in order to obtain a reconstructed droplet as compact as possible.

$$\begin{aligned} V_p &= \alpha V_d^1 + V_d^{1-f} \\ \alpha &= (V_p - V_d^{1-f})/V_d^1 \end{aligned}$$

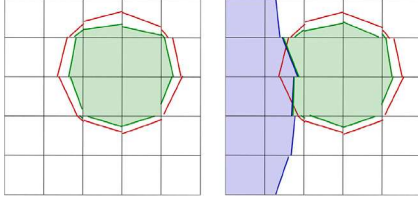


Fig. A.27. Case A: Droplet volume is over-estimated, $V_d > V_p > V_d^1 + V_d^{1-f}$. The corrections in terms of volume fractions are: $f_i^{td} = \alpha f_i^d$ in interface cells, $f_i^{td} = 1$ in filled cells, and $f_i^{td} = 1 - f_i$ in overfilled cells.

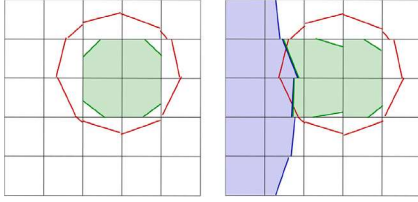


Fig. A.28. Case B: Droplet volume is over-estimated, and even $V_p < V_d^1 + V_d^{1-f}$. The corrections in terms of volume fractions are: $f_i^{td} = 0$ in interface cells, $f_i^{td} = \alpha$ in filled cells, $f_i^{td} = 1 - f_i$ in overfilled cells.

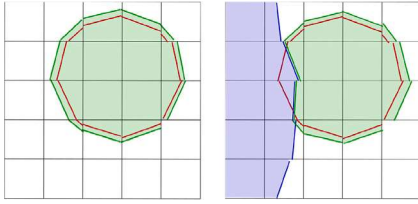


Fig. A.29. Case C: Droplet volume is under-estimated, $V_d < V_p$. The corrections in terms of volume fractions are: $f_i^{td} = 1 - \alpha(1 - f_i^d)$ in interface cells, $f_i^{td} = 1$ in filled cells, $f_i^{td} = 1 - f_i$ in overfilled cells.

A.2. Under-estimated droplet volume

Now we consider the case where the volume is under-estimated, $V_d < V_p$ (see Fig. A.29). Again, the volume fractions involved in V_d^{cor} are scaled. We define the volume fractions before and after scaling f_i^d and f_i^{td} . The strategy is now to reduce the empty parts of these cells, instead of increasing the fluid volume fraction, to avoid $f_i^{td} > 1$. The scaling reads: $1 - f_i^{td} = \alpha(1 - f_i^d)$. $\alpha > 1$ is then still valid.

- The scaled equations for this case C are given:

$$\begin{aligned}
 V_p &= \sum_{f_i^d < 1, f_i^d + f_i < 1} f_i^{td} dV_i \\
 &+ \sum_{f_i^d = 1, f_i^d + f_i < 1} f_i^d dV_i + \sum_{f_i^d < 1, f_i^d + f_i > 1} (1 - f_i) dV_i \\
 V_p &= (1 - \alpha) V_d^{cor,1} + \alpha V_d^{cor} + V_d^1 + V_d^{1-f} \\
 \text{with } V_d^{cor,1} &= \sum_{f_i^d < 1, f_i^d + f_i < 1} dV_i \text{ the sum of the cell volume in interface cells.} \\
 \text{Finally the scaling factor is found:} \\
 \alpha &= \frac{V_p - V_d^{cor,1} - V_d^1 - V_d^{1-f}}{V_d - V_d^{cor,1} - V_d^1 - V_d^f} \quad (\text{A.2})
 \end{aligned}$$

Appendix B. Budget equation for the number of droplets.

The aim of this section is to explain the difference in total number of droplets between simulations with pure DNS and DNS coupled with the Lagrangian method.

We start with the budget equation for the number of droplets. The variation of the total number of droplets (meaning all the coherent liquid structures) in the whole computation domain during a given timestep Δt reads:

$$\begin{aligned}
 \Delta N &= N_{NewFromJet} - N_{BackToJet} \\
 &+ N_{ResultFromBreakup} - N_{BrokenUp} \\
 &+ N_{ResultFromCoalescence} - N_{Merged} \\
 &- N_{LeavingAtOutflow} \quad (\text{B.1})
 \end{aligned}$$

$N_{NewFromJet}$ and $N_{BackToJet}$ are the number of structures just separated from the coherent jet corresponding to primary jet breakup, and impacting on its surface, respectively. Variations in droplet count also arise from breakup and coalescence processes. $\Delta N_{Breakup} = N_{ResultFromBreakup} - N_{BrokenUp}$ is the amount of supplementary droplets due to droplet secondary break up, whereas $\Delta N_{Coalescence} = N_{ResultFromCoalescence} - N_{Merged}$ decreases the overall number of droplets due to coalescence events. $N_{LeavingAtOutflow}$ is the number of droplets leaving the computation domain at the outflow.

If the conversion criteria fail to transfer droplets stable with respect to breakup and coalescence, this would result in a difference in number of droplets between pure VOF and coupled simulations. Consider the case where certain droplets remain stable once transferred to the Lagrangian solver, whereas in a pure DNS simulation, these droplets would have undergone coalescence. Then, the number of additional droplets during a given timestep resulting from the coupled simulations due to post-transfer coalescence events is given by $\Delta N_{Coalescence}^{(pure\ DNS)} - \Delta N_{Coalescence}^{(DNS + Lagrange)}$. A basic example is provided in Fig. B.30 for illustration.

Similarly, coupled simulations will deliver less droplets than pure DNS due to post-transfer droplet breakup.

Appendix C. Identification of droplet coalescence and breakup events.

To identify coalescence and breakup events, the list of resolved (DNS) droplets is needed. At each time step $t_0 + \Delta t$, the post-processing algorithm compares position coordinates and volumes of all resolved droplets to the ones from the preceding timestep t_0 . Droplet positions at the preceding time step are shifted by their velocity multiplied by the time step, which brings them closer to their positions at next time step. While the timestep of the Lagrangian method was set to $dt_{lag} = 5 \times 10^{-6}$ s, we observed that $\Delta t = 10^{-6}$ s is a good time difference to follow the topology changes of the droplets. The algorithm proceeds in two consecutive steps.

In the first step, we identify the droplets that are just convected between t_0 and $t_0 + \Delta t$. This is the case if they fulfill volume conservation and are “close to each other”. In practice, the difference in volume and the distance between the shifted droplets at t_0 and the droplets at $t_0 + \Delta t$ are compared with threshold values. There is a threshold for the relative change in volume and another one for the absolute distance between two droplets, respectively of the order of magnitude $O(10^{-18})$ and $O(10^{-5})$.

All the remaining droplets are then investigated in the second step. As they are not just convected, they may have experienced coalescence or breakup. We construct a so-called “connect matrix” with these remaining droplets in the following way. The column index of this matrix correspond to the shifted droplets at the old timestep t_0 (called old droplets in the following), and the row index correspond to the droplets at the new timestep $t_0 + \Delta t$ (new droplets). Initially, the matrix is populated with 0. Next, for each old droplet, a 1 is inserted in

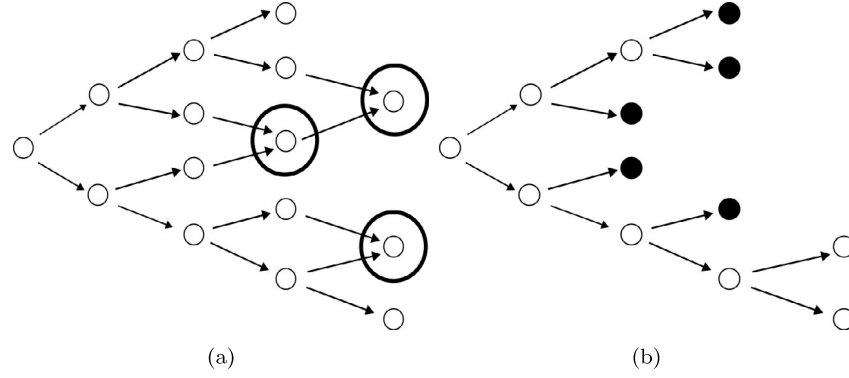


Fig. B.30. Example of a droplet's history during a given period of time, where droplets are transferred to the Lagrangian method although they would still coalesce in pure DNS simulations. The black and white droplets are respectively the Lagrangian point-droplets and the Eulerian resolved droplets. The coupled simulation (b) result in 7 droplets, whereas the pure DNS simulation (a) provide only 4 droplets. The difference of 3 droplets is exactly the number of supplementary droplets resulting from post-transfer coalescence processes encircled in subfigure (a).

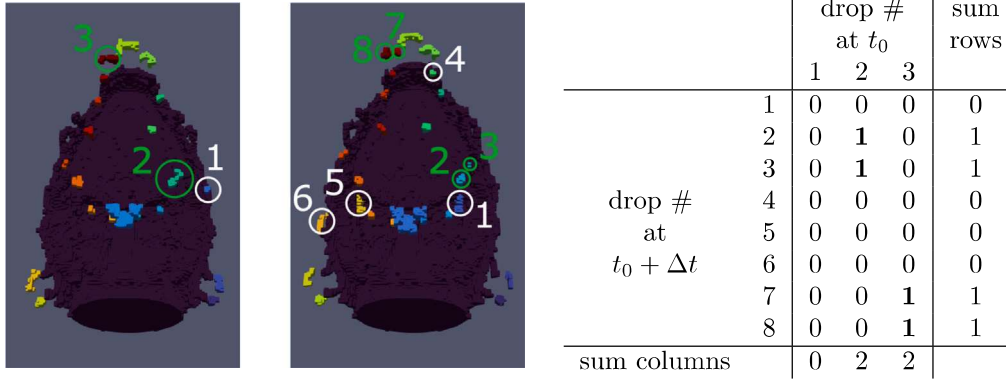


Fig. C.31. Example with two breakup events between $t_0 = 3.2 \times 10^{-5}$ s (left figure) and $t_0 + \Delta t$ (right figure).

the matrix at the position of the nearest new droplet (task 1): This determines the nearest new drop (only one) created from the old drop. The procedure is repeated for all new droplets, whereby the value 1 is inserted in the matrix at the position of the nearest old droplet (task 2): This determines the nearest old droplet (also only one) from which the new one was created. These two last steps are performed only if the distance between the two nearest droplets is smaller than a previously established cutoff of the order of magnitude $O(10^{-4})$. We do not identify a-priori the coalescence and breakup events applying the described procedure (set the values 1), these events are obtained automatically from the observation of the resulting matrix.

This happens in the following way. If the sum over a column strictly exceeds 1, we have an indication for a potential breakup (several new droplets are created from the same old droplet), or a potential coalescence in the case of a row (a new droplets is created from several old droplet). Finally, we check the volume conservation to validate the identification of breakup and coalescence events trying all the potential droplets combinations for which the value 1 is filled in for a given column or a given row respectively. It is also possible that the volume does not match for any combination, meaning the old droplet is the nearest to the identified new droplet, but the volume difference exceeds the defined threshold. This happens for example near the jet, when fractions of liquid separate from the jet and combine with already existing droplets.

Other situations may also occur: If the sum of all the matrix elements of a given column corresponding to a old drop is 0, this drop is far away from every new drop, from which it is interpreted that it has merged back into the liquid jet, as it is the case in Fig. C.31 for drop #1 at t_0 . Similarly, in the case a row adds up to 0, the corresponding new

drop is just separated from the coherent jet, as is the case for drops # 1, 4, 5, 6 at $t_0 + \Delta t$ in Fig. C.31.

For the early atomization of jet A-1 in the case U75q2, we present examples with two breakup processes in Fig. C.31 and with four coalescence events in Fig. C.32 and in Table C.5 (the corresponding connect matrix). Pure DNS simulations were conducted with a maximum level of refinement of 12 for the VOF variable and 10 for the velocity field. After filtering out the droplets that are just convected (first step of the algorithm), the remaining ones (encircled in the figures) are used to construct the connect matrix (second step). The corresponding connect matrix in the case of two breakup processes (Fig. C.31) indicates that drops #2 and #3 at t_0 break up respectively in drops # (2,3) and drops # (7,8) at $t_0 + \Delta t$. As previously explained, in the context of task 2, we find that the old droplet closest to the new droplets 7 and 8 is 3 in both cases. Thus, from the observation of the obtained matrix, we can see that the old droplet 3 potentially breaks up into the new droplets 7 and 8. Finally, the conservation of volume is checked to confirm the breakup process. Drop #1 at t_0 returns to the jet, and drops # 1, 4, 5, 6 at $t_0 + \Delta t$ are just generated from the jet. In the case of four coalescence events (in Fig. C.32 and Table C.5), the outcome of the post-processing algorithm is the following: Drops # 4, 5, 6, 7 at $t_0 + \Delta t$ are the result of coalescence events between respectively drops # (5,14), (6,7), (8,9), (1,2) at t_0 . Drops # 11, 12 at t_0 return to the jet. New drops at $t_0 + \Delta t$ are: 1, 9, 11, 12. The method does not identify a breakup of drop # 10 in #(8,9,12). The ligaments are probably too far away from each other, and it could be that new volume of liquid was added due to the proximity of the jet.

The post-processing method presented depends on the threshold values used to evaluate the volume conservation and proximity between droplets. Both thresholds are set to validate breakup and coalescence

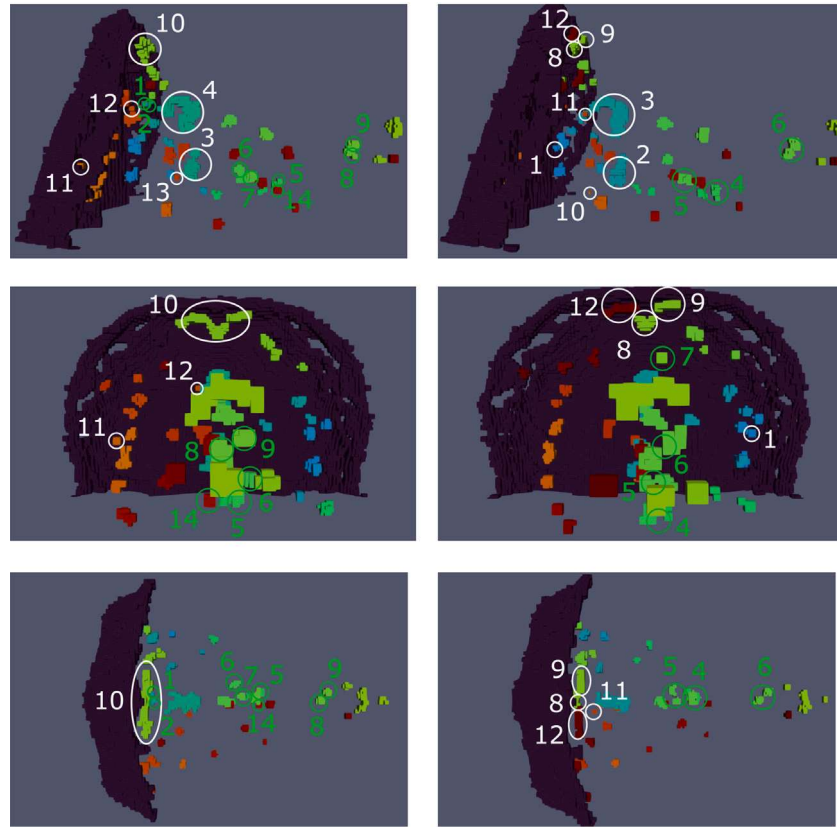


Fig. C.32. Example of four coalescence phenomena. The figures show different views at $t_0 = 4.6 \times 10^{-5}$ s (on the left) and $t_0 + \Delta t$ (on the right).

Table C.5

Connect matrix corresponding to Fig. C.32 including four coalescence processes at $t_0 = 4.6 \times 10^{-5}$ s.

		drops at t_0														sum rows
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	
drops at $t_0 + \Delta t$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1
	3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1
	4	0	0	0	0	1	0	0	0	0	0	0	0	0	1	2
	5	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2
	6	0	0	0	0	0	0	0	1	1	0	0	0	0	0	2
	7	1	1	0	0	0	0	0	0	0	0	0	0	0	0	2
	8	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1
	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	10	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1
	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sum columns		1	1	1	1	1	1	1	1	1	1	0	0	1	1	

events during the early stages of atomization, where every event can be tracked by visualization. At a later stage of the atomization, when droplet number becomes large, the method is effective in identifying the majority of coalescence and breakup events, and therefore regions with a high density of merging events.

See Table C.5.

Appendix D. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.compfluid.2026.107230>.

Data availability

The authors are unable or have chosen not to specify which data has been used.

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